

An Experimental and Modeling Study of Propene Oxidation. Part 1: Speciation Measurements in Jet-Stirred and Flow Reactors.

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Jet-stirred reactor data

Table 1 Experimental data from Nancy JSR: 1.65% C₃H₆ 11.60% O₂ 86.75% He, $\phi=0.64$, $p=1.05$ atm, $\tau=2.0$ s.

Mole Fraction									
T, K	O ₂	CO	CO ₂	CH ₄	C ₂ H ₄	C ₂ H ₂	C ₂ H ₆	C ₃ H ₆	CH ₃ CHO
800	1.16E-01			1.79E-05	3.12E-05			1.65E-02	1.25E-05
825	1.18E-01	3.93E-05		1.85E-05	2.90E-05			1.63E-02	1.69E-05
850	1.14E-01	1.19E-04	8.19E-05	2.16E-05	6.37E-05			1.64E-02	4.82E-05
875	1.12E-01	9.35E-04	1.36E-04	1.47E-04	4.63E-04		3.63E-06	1.55E-02	2.07E-04
900	9.65E-02	1.23E-02	1.26E-03	1.25E-03	3.31E-03		6.47E-05	6.92E-03	4.18E-04
950	7.98E-02	2.28E-02	3.88E-03	1.60E-03	3.75E-03		8.88E-05	3.28E-03	2.95E-04
925	8.64E-02	2.08E-02	2.56E-03	1.55E-03	3.39E-03		8.35E-05	2.07E-03	2.07E-04
975	7.23E-02	5.83E-03	1.79E-02	9.25E-04	1.47E-03	2.99E-06	5.15E-05	5.84E-04	6.86E-05
1000	6.35E-02	2.68E-03	2.61E-02	4.35E-04	1.14E-03	1.55E-05	4.13E-05	6.01E-04	1.37E-04
1025	5.52E-02	2.86E-03	3.15E-02	4.11E-04	1.06E-03	1.99E-05	4.59E-05	1.83E-03	2.44E-05
1050	4.31E-02	5.28E-03	3.55E-02	1.56E-04	3.12E-04	1.96E-05	1.75E-05	3.05E-04	2.24E-05
1075	3.81E-02	2.98E-03	4.15E-02	1.15E-04	2.32E-04	1.40E-05	1.55E-05	2.90E-04	
1085		8.58E-05		9.79E-05	2.03E-04		1.31E-05	2.49E-04	
T, K	C ₄ H ₈	C ₄ H ₆	C ₃ H ₆ O1-2	C ₂ H ₃ CHO	C ₂ H ₅ CHO	CH ₃ COCH ₃	C ₆ H ₁₀	C ₆ H ₆	
800	2.88E-06			4.55E-06	3.30E-06	5.78E-06	3.54E-06	1.01E-05	
825	3.86E-06		6.93E-06	1.49E-05		8.12E-06	1.36E-05	1.13E-05	
850	1.55E-05	2.61E-06	1.12E-05	2.43E-05	1.52E-05	5.78E-06	2.30E-05	1.24E-05	
875	1.00E-04	1.35E-05	3.53E-05	1.41E-04	6.30E-05	2.44E-05	5.42E-05	1.38E-05	
900	1.81E-04	4.41E-05	7.62E-05	3.06E-04	8.38E-05	6.73E-05	2.18E-05	1.71E-05	
950	9.50E-05	2.66E-05	2.55E-05	1.87E-04	3.96E-05	6.31E-05	7.62E-06	1.52E-05	
925	5.97E-05	1.72E-05	2.87E-05	1.11E-04	2.54E-05	3.63E-05	2.58E-06	1.23E-05	
975	1.69E-05	4.34E-06	1.47E-05	2.71E-05	5.61E-06	4.62E-05			
1000	1.64E-05	4.38E-06	5.61E-06	2.67E-05	5.45E-06	1.19E-05		9.10E-06	
1025	1.61E-05	7.12E-06		1.46E-05		6.93E-06		8.58E-06	
1050	1.61E-05	7.99E-06							
1075				1.47E-05		5.28E-06		1.09E-05	
1085	1.47E-05	7.99E-06		1.22E-05		1.62E-05		9.74E-06	

**Table 2 Experimental data from Nancy JSR: 1.62% C₃H₆ 6.81% O₂ 91.57% He, $\phi=1.07$,
 $p=1.05$ atm, $\tau=2.0$ s.**

Mole Fraction									
T, K	O ₂	CO	CO ₂	CH ₄	C ₂ H ₄	C ₂ H ₂	C ₂ H ₆	C ₃ H ₆	CH ₃ CHO
800	6.81E-02							1.62E-02	
825	6.79E-02	2.15E-05			6.74E-06			1.63E-02	7.92E-06
850	6.73E-02	4.13E-05		1.05E-05	2.12E-05			1.61E-02	1.65E-05
875	6.69E-02	1.26E-04		3.56E-05	8.32E-05			1.60E-02	4.36E-05
900	6.80E-02	5.37E-04	2.70E-04	1.26E-04	3.15E-04			1.53E-02	9.64E-05
925	5.01E-02	1.28E-02	1.26E-03	1.58E-03	3.69E-03		9.93E-05	5.89E-03	3.48E-04
950	4.07E-02	1.87E-02	2.80E-03	2.01E-03	4.18E-03	4.62E-06	1.31E-04	3.57E-03	2.61E-04
975	3.72E-02	2.12E-02	4.01E-03	2.22E-03	4.05E-03	8.43E-06	1.47E-04	2.27E-03	1.38E-04
1000	3.53E-02	2.25E-02	4.55E-03	2.36E-03	3.74E-03	9.25E-06	1.59E-04	1.52E-03	8.91E-05
1025	3.19E-02	2.36E-02	5.17E-03	2.32E-03	3.10E-03	1.14E-05	1.55E-04	9.84E-04	1.03E-04
T, K	C ₄ H ₈	C ₄ H ₆	C ₃ H ₆ O1-2	C ₂ H ₃ CHO	C ₂ H ₅ CHO	CH ₃ COCH ₃	C ₆ H ₁₀	C ₆ H ₆	
800			6.01E-06	6.32E-06		3.30E-06	3.32E-06	1.07E-05	
825	1.86E-06		3.30E-06	6.95E-06		3.30E-06	4.67E-06	8.67E-06	
850	4.23E-06		3.63E-06	1.39E-05	4.29E-06		1.17E-05	7.84E-06	
875	2.10E-05	2.95E-06	6.27E-06	3.03E-05	1.29E-05	4.95E-06	2.41E-05	8.32E-06	
900	8.39E-05	1.13E-05	1.02E-05	1.00E-04	4.36E-05	1.39E-05	3.92E-05	1.05E-05	
925	2.11E-04	5.25E-05	3.37E-05	3.05E-04	7.36E-05	6.24E-05	1.18E-05	1.66E-05	
950	1.39E-04	4.12E-05	1.49E-05	1.12E-04	4.42E-05	5.28E-05	3.93E-06	1.44E-05	
975	8.97E-05	3.18E-05	3.30E-06	1.71E-04	2.77E-05	3.86E-05		1.25E-05	
1000	6.11E-05	2.48E-05		5.97E-05	1.82E-05	2.41E-05		1.01E-05	
1025	3.91E-05	1.84E-05		3.16E-05	1.02E-05	4.29E-06	1.23E-06	1.01E-05	

**Table 3 Experimental data from Nancy JSR: 1.68% C₃H₆ 4.50% O₂ 93.82% He, $\phi=1.68$,
 $p=1.05$ atm, $\tau=2.0$ s.**

Mole Fraction									
T, K	O ₂	CO	CO ₂	CH ₄	C ₂ H ₄	C ₂ H ₂	C ₂ H ₆	C ₃ H ₆	CH ₃ CHO
800	4.50E-02	1.77E-05						1.68E-02	
850	4.21E-02	2.69E-05			1.11E-05			1.73E-02	9.24E-06
875	4.36E-02	6.40E-05		1.85E-05	3.71E-05			1.63E-02	2.11E-05
900	4.03E-02	1.79E-04		5.05E-05	9.80E-05			1.58E-02	3.52E-05
925	3.88E-02	4.94E-04		1.52E-04	3.21E-04			1.57E-02	1.07E-04
950	3.64E-02	1.65E-03	1.33E-04	4.44E-04	9.21E-04	2.99E-06	8.12E-06	1.37E-02	3.01E-04
975	2.90E-02	7.98E-03	4.16E-04	1.91E-03	3.51E-03	1.55E-05	9.11E-05	7.99E-03	3.01E-04
1000	2.81E-02	1.10E-02	1.09E-03	2.75E-03	4.52E-03	1.99E-05	1.44E-04	6.21E-03	2.83E-04
1025	2.31E-02	1.18E-02	1.35E-03	3.61E-03	5.14E-03	1.96E-05	1.86E-04	5.04E-03	2.18E-04
1050	2.17E-02	1.54E-02	2.07E-03	4.44E-03	5.55E-03	1.40E-05	2.44E-04	3.17E-03	1.59E-04
1075	1.85E-02	1.64E-02	2.31E-03	5.51E-03	5.90E-03		2.84E-04	2.54E-03	1.23E-04
1100	1.50E-02	1.80E-02	2.24E-03	6.18E-03	5.47E-03	3.78E-05	2.93E-04	1.51E-03	8.05E-05
T, K	C ₃ H _{4-a}	C ₃ H _{4-p}	C ₄ H ₈	C ₄ H ₆	C ₂ H ₃ CHO	C ₂ H ₅ CHO	CH ₃ COCH ₃	C ₆ H ₁₀	C ₆ H ₆
800			0.00E+00		8.68E-06		6.93E-06	1.47E-06	
850			2.88E-06		1.18E-05		5.12E-06	7.50E-06	
875			1.07E-05	2.43E-06	1.29E-05	7.59E-06	8.91E-06	1.70E-05	9.98E-06
900			2.95E-05	4.86E-06	3.27E-05	1.06E-05	9.90E-06	1.97E-05	9.98E-06
925	4.00E-06		1.03E-04	1.61E-05	7.82E-05	3.85E-05	1.62E-05	2.97E-05	1.14E-05
950	9.69E-06		2.37E-04	4.97E-05	1.85E-04	7.00E-05	3.07E-05	2.54E-05	1.46E-05
975	1.06E-05	6.64E-06	3.72E-04	1.43E-04	2.80E-04	9.24E-05	6.45E-05	9.43E-06	1.85E-05
1000	1.49E-05	1.11E-05	3.28E-04	1.60E-04	2.37E-04	7.23E-05	6.57E-05	7.50E-06	1.82E-05

Table 4 Experimental data from Nancy JSR: 1.68% C₃H₆ 4.50% O₂ 93.82% He, $\phi=1.68$, $p=1.05$ atm, $\tau=2.0$ s.

Mole Fraction									
T, K	O ₂	CO	CO ₂	CH ₄	C ₂ H ₄	C ₂ H ₂	C ₂ H ₆	C ₃ H ₆	CH ₃ CHO
800	3.41E-02	1.59E-05						1.64E-02	
825	3.33E-02							1.62E-02	7.66E-06
850	3.40E-02	2.09E-05			7.08E-06			1.63E-02	1.39E-05
875	3.34E-02	5.43E-05		1.60E-05	2.66E-05			1.62E-02	6.80E-06
900	3.31E-02	8.78E-05		3.88E-05	7.11E-05			1.60E-02	2.66E-05
925	3.41E-02	3.63E-04		9.98E-05	2.03E-04			1.49E-02	5.74E-05
950	3.17E-02	9.43E-04		2.91E-04	5.81E-04		2.74E-05	1.47E-02	1.14E-04
975	3.08E-02	3.07E-03	3.95E-04	9.41E-04	1.78E-03			1.19E-02	2.13E-04
1000	2.50E-02	6.33E-03	4.37E-04	2.01E-03	3.35E-03	3.54E-06	8.05E-05	8.56E-03	2.45E-04
1025	2.25E-02	8.84E-03	9.24E-04	3.02E-03	4.45E-03	4.62E-06	1.35E-04	6.87E-03	2.20E-04
1050	2.00E-02	1.14E-02	1.61E-03	4.19E-03	5.39E-03	1.77E-05	2.12E-04	4.44E-03	1.72E-04
1085	1.67E-02	1.56E-02	2.47E-03	5.56E-03	5.68E-03	1.03E-05	2.85E-04	2.37E-03	9.70E-05
1100	1.43E-02	1.72E-02	2.59E-03	6.24E-03	5.54E-03	9.10E-05	2.97E-04	1.68E-03	7.26E-05
T, K	C ₃ H ₄ -a	C ₃ H ₄ -p	C ₄ H ₈	C ₄ H ₆	C ₂ H ₃ CHO	C ₂ H ₅ CHO	CH ₃ COCH ₃	C ₆ H ₁₀	C ₆ H ₆
800					6.74E-06		1.98E-05	1.84E-06	1.03E-05
825			1.69E-06		6.60E-06		4.95E-06	5.04E-06	1.03E-05
850			1.93E-06		8.68E-06		6.60E-06	1.16E-05	9.38E-06
875			7.11E-06	1.82E-06	1.34E-05	4.62E-06	3.86E-06	1.76E-05	8.20E-06
900			2.17E-05	4.86E-06	2.54E-05	6.93E-06	8.15E-06	2.15E-05	9.15E-06
925			6.90E-05	1.01E-05	5.91E-05	2.24E-05	1.22E-05		1.06E-05
950	8.46E-06		1.76E-04	3.23E-05	1.45E-04	4.75E-05	1.78E-05	2.37E-05	1.23E-05
975	2.00E-05		3.58E-04	1.09E-04	2.81E-04	8.12E-05	4.39E-05	1.63E-05	9.27E-06
1000	2.33E-05	3.61E-06	3.81E-04	1.76E-04	2.67E-04	7.59E-05	7.59E-05	8.48E-06	2.50E-05
1025	3.20E-05	5.36E-06	3.31E-04	1.99E-04	2.06E-04	5.68E-05	3.80E-05	4.55E-06	3.80E-05
1050	3.80E-05	1.36E-05	2.14E-04	1.63E-04	1.21E-04	3.29E-05	2.57E-05	1.97E-06	4.62E-05
1085	4.02E-05	3.07E-05	1.04E-04	9.95E-05	5.18E-05	1.39E-05	1.19E-05		5.02E-05
1100	3.77E-05	3.44E-05	7.04E-05	7.45E-05	3.47E-05	6.27E-06	9.24E-06		5.29E-05

Flow reactor data

Princeton Variable pressure flow reactor data

Table 5 VPFR Experimental data: 0.33% C₃H₆ 2.10% O₂ 97.57% N₂, $\phi=0.71$, $p=6$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
4.32E-02	9.70E+02	2.08E-02	3.60E-05	1.34E-04	3.19E-03	2.46E-04	3.66E-06	4.01E-05	3.03E-05
9.92E-02	9.66E+02	2.05E-02	5.56E-05	2.22E-04	3.04E-03	3.68E-04	3.90E-05	6.33E-05	5.23E-05
1.38E-01	9.67E+02	2.05E-02	5.60E-05	2.80E-04	2.95E-03	4.15E-04	5.65E-05	8.52E-05	6.80E-05
1.81E-01	9.67E+02	2.04E-02	6.37E-05	3.45E-04	2.86E-03	5.21E-04	6.67E-05	1.16E-04	8.32E-05
2.28E-01	9.68E+02	2.02E-02	6.76E-05	4.77E-04	2.71E-03	6.45E-04	8.58E-05	1.60E-04	1.10E-04
2.74E-01	9.70E+02	2.00E-02	7.70E-05	6.22E-04	2.57E-03	7.71E-04	1.26E-04	2.48E-04	1.33E-04
3.21E-01	9.72E+02	1.97E-02	8.90E-05	8.87E-04	2.32E-03	9.52E-04	2.04E-04	4.05E-04	1.67E-04
3.68E-01	9.75E+02	1.92E-02	1.12E-04	1.28E-03	2.04E-03	1.17E-03	2.93E-04	5.61E-04	2.01E-04
4.15E-01	9.84E+02	1.82E-02	1.87E-04	2.10E-03	1.57E-03	2.37E-03	4.09E-04	6.96E-04	2.34E-04
4.61E-01	1.00E+03	1.69E-02	3.30E-04	3.29E-03	1.06E-03	3.56E-03	5.21E-04	7.83E-04	2.44E-04
5.06E-01	1.02E+03	1.50E-02	6.59E-04	4.71E-03	5.48E-04	5.19E-03	6.12E-04	7.27E-04	2.02E-04
5.51E-01	1.04E+03	1.36E-02	1.01E-03	5.67E-03	2.73E-04	6.62E-03	6.11E-04	5.63E-04	1.51E-04
5.96E-01	1.06E+03	1.18E-02	1.72E-03	6.33E-03	9.90E-05	7.63E-03	5.42E-04	4.29E-04	8.24E-05

Table 6 VPFR Experimental data: 0.33% C₃H₆ 1.48% O₂ 98.19% N₂, $\phi=1.00$, $p=6$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
2.30E-02	1.02E+03	1.45E-02	7.08E-05	1.60E-04	3.36E-03	3.34E-04	0.00E+00	5.09E-05	2.86E-05
6.35E-02	1.02E+03	1.42E-02	1.23E-04	2.70E-04	3.25E-03	4.77E-04	5.95E-05	9.03E-05	4.99E-05
1.30E-01	1.02E+03	1.40E-02	1.33E-04	4.16E-04	3.05E-03	6.41E-04	9.97E-05	1.66E-04	8.04E-05
2.16E-01	1.02E+03	1.37E-02	1.49E-04	6.13E-04	2.73E-03	8.01E-04	1.42E-04	2.45E-04	1.17E-04
2.60E-01	1.02E+03	1.36E-02	1.51E-04	7.33E-04	2.59E-03	8.89E-04	1.85E-04	3.24E-04	1.40E-04
3.05E-01	1.02E+03	1.33E-02	1.81E-04	9.18E-04	2.44E-03	9.64E-04	2.34E-04	4.05E-04	1.59E-04
3.49E-01	1.02E+03	1.31E-02	1.63E-04	1.11E-03	2.21E-03	1.11E-03	2.72E-04	4.88E-04	1.81E-04
3.94E-01	1.03E+03	1.26E-02	1.83E-04	1.56E-03	1.78E-03	1.40E-03	4.00E-04	6.79E-04	2.12E-04
4.38E-01	1.03E+03	1.21E-02	2.12E-04	2.01E-03	1.48E-03	1.89E-03	4.74E-04	8.19E-04	2.34E-04
4.83E-01	1.04E+03	1.13E-02	2.76E-04	2.80E-03	1.06E-03	2.50E-03	6.16E-04	9.61E-04	2.45E-04
5.27E-01	1.05E+03	9.96E-03	4.47E-04	3.91E-03	6.00E-04	3.64E-03	7.40E-04	1.03E-03	2.21E-04
5.70E-01	1.06E+03	8.75E-03	6.88E-04	4.77E-03	4.31E-04	4.72E-03	7.65E-04	9.90E-04	1.84E-04
6.14E-01	1.08E+03	6.65E-03	1.57E-03	5.55E-03	1.79E-04	6.17E-03	5.96E-04	6.15E-04	1.09E-04

Table 7 VPFR Experimental data: 0.33% C₃H₆ 2.14% O₂ 97.53% N₂, $\phi=0.71$, $p=8$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
1.50E-02	9.15E+02	2.08E-02	3.65E-05	7.81E-05	3.36E-03	1.70E-04	0.00E+00	0.00E+00	1.71E-05
3.52E-02	9.17E+02	2.07E-02	4.10E-05	9.06E-05	3.33E-03	1.98E-04	0.00E+00	0.00E+00	2.09E-05
6.09E-02	9.15E+02	2.07E-02	3.79E-05	1.08E-04	3.28E-03	2.17E-04	0.00E+00	0.00E+00	2.58E-05
9.54E-02	9.16E+02	2.06E-02	4.96E-05	1.40E-04	3.19E-03	2.62E-04	0.00E+00	3.25E-05	3.38E-05
1.40E-01	9.16E+02	2.06E-02	5.43E-05	1.70E-04	3.17E-03	3.10E-04	0.00E+00	4.53E-05	4.32E-05
1.94E-01	9.16E+02	2.05E-02	6.64E-05	2.16E-04	3.16E-03	3.75E-04	0.00E+00	5.65E-05	5.41E-05
2.55E-01	9.20E+02	2.06E-02	5.77E-05	2.81E-04	3.02E-03	4.56E-04	5.01E-05	8.32E-05	7.40E-05
3.20E-01	9.22E+02	2.03E-02	7.01E-05	4.39E-04	2.83E-03	6.30E-04	5.97E-05	1.16E-04	1.06E-04
3.86E-01	9.22E+02	2.02E-02	7.90E-05	5.70E-04	2.66E-03	7.61E-04	8.75E-05	1.83E-04	1.32E-04
4.51E-01	9.30E+02	1.92E-02	9.75E-05	8.25E-04	2.42E-03	9.40E-04	1.14E-04	2.62E-04	1.68E-04
5.16E-01	9.40E+02	1.70E-02	3.07E-04	1.60E-03	1.98E-03	2.02E-03	2.12E-04	4.81E-04	2.36E-04
5.79E-01	9.54E+02	1.50E-02	6.00E-04	3.29E-03	1.38E-03	3.08E-03	3.00E-04	6.98E-04	2.09E-04
7.06E-01	9.82E+02	1.38E-02	8.75E-04	5.38E-03	4.12E-04	6.10E-03	4.53E-04	7.11E-04	1.60E-04

Table 8 VPFR Experimental data: 0.31% C₃H₆ 1.49% O₂ 98.20% N₂, $\phi=0.94$, $p=8$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
1.41E-02	9.54E+02	1.49E-02	5.08E-05	1.08E-04	3.00E-03	2.18E-04	3.66E-06	1.20E-05	1.80E-05
5.71E-02	9.56E+02	1.47E-02	9.17E-05	2.00E-04	2.99E-03	3.77E-04	3.66E-06	3.77E-05	2.95E-05
1.31E-01	9.55E+02	1.46E-02	1.09E-04	2.88E-04	2.85E-03	4.84E-04	4.25E-05	6.79E-05	4.89E-05
2.39E-01	9.58E+02	1.43E-02	1.26E-04	4.80E-04	2.57E-03	6.83E-04	8.00E-05	1.57E-04	9.09E-05
3.62E-01	9.64E+02	1.38E-02	1.61E-04	9.36E-04	2.20E-03	1.02E-03	1.53E-04	3.28E-04	1.47E-04
4.23E-01	9.66E+02	1.31E-02	1.95E-04	1.47E-03	1.85E-03	1.46E-03	2.40E-04	4.87E-04	1.85E-04
4.84E-01	9.77E+02	1.17E-02	3.30E-04	2.75E-03	1.24E-03	2.53E-03	4.21E-04	7.42E-04	2.12E-04
5.45E-01	9.93E+02	9.92E-03	5.80E-04	4.29E-03	6.56E-04	3.93E-03	4.85E-04	7.95E-04	1.93E-04
6.04E-01	1.02E+03	8.27E-03	9.47E-04	5.47E-03	3.01E-04	5.28E-03	5.69E-04	7.62E-04	1.33E-04
6.62E-01	1.03E+03	6.68E-03	1.48E-03	6.20E-03	1.06E-04	5.97E-03	5.76E-04	5.21E-04	6.75E-05
7.20E-01	1.04E+03	5.95E-03	1.85E-03	6.45E-03	4.50E-05	6.06E-03	5.32E-04	3.66E-04	4.58E-05
7.78E-01	1.04E+03	5.11E-03	2.35E-03	6.47E-03	1.86E-05	6.39E-03	3.87E-04	1.45E-04	2.92E-05
8.36E-01	1.06E+03	4.22E-03	3.19E-03	6.12E-03	1.09E-05	6.56E-03	1.89E-04	3.82E-05	1.62E-05

Table 9 VPFR Experimental data: 0.33% C₃H₆ 1.13% O₂ 98.54% N₂, $\phi=1.31$ $p=8$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	C ₂ H ₄	CH ₄	CH ₂ O
1.37E-02	9.88E+02	1.11E-02	5.25E-05	1.40E-04	3.16E-03	2.51E-04	3.82E-05	3.66E-06	2.57E-05
5.54E-02	9.87E+02	1.09E-02	6.97E-05	2.31E-04	3.07E-03	3.74E-04	6.07E-05	4.17E-05	4.27E-05
1.28E-01	9.82E+02	1.07E-02	9.84E-05	3.48E-04	2.89E-03	5.35E-04	1.07E-04	6.29E-05	6.52E-05
2.33E-01	9.83E+02	1.06E-02	1.13E-04	4.83E-04	2.71E-03	6.68E-04	1.65E-04	9.73E-05	9.23E-05
3.53E-01	9.87E+02	1.02E-02	1.29E-04	7.73E-04	2.40E-03	8.50E-04	3.20E-04	1.80E-04	1.38E-04
4.13E-01	9.86E+02	9.95E-03	1.40E-04	9.80E-04	2.21E-03	9.46E-04	3.91E-04	2.18E-04	1.60E-04
4.74E-01	9.90E+02	9.49E-03	1.58E-04	1.37E-03	1.86E-03	1.24E-03	5.24E-04	2.91E-04	1.93E-04
5.34E-01	9.94E+02	9.10E-03	1.96E-04	1.73E-03	1.62E-03	1.51E-03	7.35E-04	4.27E-04	2.11E-04
5.94E-01	1.00E+03	8.27E-03	2.28E-04	2.49E-03	1.19E-03	2.31E-03	9.03E-04	5.61E-04	2.32E-04
6.53E-01	1.01E+03	7.14E-03	3.35E-04	3.48E-03	7.55E-04	3.23E-03	1.06E-03	6.77E-04	2.27E-04
7.13E-01	1.02E+03	6.18E-03	4.38E-04	4.31E-03	4.55E-04	4.10E-03	1.13E-03	8.47E-04	2.06E-04
7.71E-01	1.03E+03	4.92E-03	6.52E-04	5.40E-03	1.88E-04	5.38E-03	1.07E-03	9.34E-04	1.51E-04
8.30E-01	1.04E+03	3.91E-03	8.36E-04	6.15E-03	9.04E-05	5.95E-03	7.39E-04	7.41E-04	1.05E-04

Table 10 VPFR Experimental data: 0.33% C₃H₆ 2.14% O₂ 97.53% N₂, $\phi=0.70$ $p=10$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
1.92E-02	8.76E+02	2.07E-02	3.10E-05	5.46E-05	3.32E-03	1.10E-04	3.66E-06	1.20E-05	1.12E-05
7.75E-02	8.74E+02	2.06E-02	4.87E-05	1.03E-04	3.27E-03	1.99E-04	3.66E-06	1.20E-05	2.17E-05
1.78E-01	8.70E+02	2.07E-02	7.26E-05	1.68E-04	3.20E-03	3.04E-04	3.66E-06	1.20E-05	3.39E-05
3.26E-01	8.71E+02	2.06E-02	7.99E-05	2.32E-04	3.13E-03	3.89E-04	3.66E-06	5.18E-05	5.39E-05
4.93E-01	8.72E+02	2.05E-02	8.50E-05	3.25E-04	2.99E-03	5.12E-04	4.05E-05	8.41E-05	8.58E-05
5.78E-01	8.72E+02	2.04E-02	8.96E-05	3.91E-04	2.92E-03	5.91E-04	5.79E-05	1.28E-04	1.04E-04
7.46E-01	8.85E+02	1.89E-02	1.95E-04	1.78E-03	2.38E-03	1.75E-03	1.63E-04	3.62E-04	1.97E-04
8.28E-01	9.06E+02	1.67E-02	4.95E-04	3.67E-03	1.79E-03	3.04E-03	2.82E-04	5.87E-04	3.04E-04
9.09E-01	9.26E+02	1.46E-02	7.73E-04	5.11E-03	1.08E-03	4.80E-03	3.91E-04	6.38E-04	2.07E-04
9.89E-01	9.50E+02	1.33E-02	1.02E-03	6.04E-03	4.05E-04	6.29E-03	5.21E-04	6.40E-04	1.18E-04
1.07E+00	9.66E+02	1.21E-02	1.36E-03	6.83E-03	1.72E-04	7.46E-03	5.47E-04	5.94E-04	1.00E-04
1.15E+00	9.82E+02	1.06E-02	2.05E-03	7.36E-03	3.48E-05	7.69E-03	3.93E-04	2.93E-04	7.18E-05
1.22E+00	9.89E+02	1.01E-02	2.27E-03	7.40E-03	2.44E-05	7.83E-03	1.96E-04	1.83E-04	4.89E-05

Table 11 VPFR Experimental data: 0.33% C₃H₆ 1.49% O₂ 98.18% N₂, $\phi=1.00$ $p=10$ atm.

Mole Fraction									
Time, s	T, K	C ₃ H ₆	CO ₂	CO	CO	H ₂ O	C ₂ H ₄	CH ₄	CH ₂ O
1.86E-02	9.12E+02	3.33E-03	1.44E-02	1.10E-04	1.43E-04	2.91E-04	3.66E-05	0.00E+00	2.85E-05
7.49E-02	9.12E+02	3.19E-03	1.46E-02	1.40E-04	2.41E-04	4.34E-04	4.71E-05	0.00E+00	4.52E-05
1.72E-01	9.09E+02	2.95E-03	1.41E-02	1.57E-04	4.84E-04	6.91E-04	1.32E-04	6.63E-05	8.18E-05
3.14E-01	9.14E+02	2.53E-03	1.41E-02	2.04E-04	9.90E-04	1.11E-03	2.44E-04	1.28E-04	1.32E-04
4.73E-01	9.32E+02	1.56E-03	1.23E-02	3.78E-04	2.57E-03	2.73E-03	4.65E-04	2.71E-04	1.95E-04
6.29E-01	9.55E+02	7.12E-04	1.03E-02	7.65E-04	4.55E-03	5.93E-03	6.26E-04	5.27E-04	1.21E-04
7.06E-01	9.73E+02	2.51E-04	8.42E-03	1.29E-03	5.93E-03	6.45E-03	5.16E-04	5.54E-04	1.00E-04
7.82E-01	9.91E+02	8.37E-05	7.25E-03	1.72E-03	6.53E-03	6.61E-03	3.98E-04	5.39E-04	7.70E-05
8.57E-01	1.00E+03	1.51E-05	6.33E-03	2.32E-03	6.64E-03	6.91E-03	2.17E-04	5.00E-04	5.15E-05
9.31E-01	1.01E+03	1.26E-05	5.95E-03	2.48E-03	6.67E-03	7.21E-03	1.33E-04	4.50E-04	3.47E-05
1.01E+00	1.02E+03	8.50E-06	5.51E-03	2.69E-03	6.61E-03	7.69E-03	1.14E-04	4.33E-04	2.57E-05
1.08E+00	1.02E+03	4.70E-06	5.40E-03	3.05E-03	6.42E-03	8.02E-03	5.38E-05	3.93E-04	2.00E-05
1.16E+00	1.02E+03	4.00E-06	5.06E-03	3.34E-03	6.20E-03	8.10E-03	3.91E-05	3.48E-04	1.60E-05

Table 12 VPFR Experimental data: 0.34% C₃H₆ 1.10% O₂ 98.56% N₂, $\phi=1.37$ $p=10$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
1.79E-02	9.44E+02	1.08E-02	1.25E-04	2.23E-04	3.35E-03	4.03E-04	3.66E-06	4.15E-05	3.36E-05
7.26E-02	9.43E+02	1.06E-02	1.64E-04	3.79E-04	3.21E-03	6.20E-04	5.58E-05	9.62E-05	5.44E-05
1.67E-01	9.42E+02	1.03E-02	2.24E-04	6.50E-04	3.02E-03	8.78E-04	1.01E-04	1.78E-04	8.99E-05
2.31E-01	9.43E+02	1.00E-02	2.51E-04	8.09E-04	2.71E-03	1.00E-03	1.31E-04	2.35E-04	1.10E-04
3.05E-01	9.48E+02	9.36E-03	3.09E-04	1.36E-03	2.26E-03	1.45E-03	2.49E-04	4.19E-04	1.48E-04
3.81E-01	9.56E+02	8.49E-03	3.77E-04	2.13E-03	1.99E-03	2.21E-03	2.95E-04	5.40E-04	1.82E-04
4.59E-01	9.63E+02	7.43E-03	4.73E-04	3.05E-03	1.42E-03	3.16E-03	4.42E-04	7.23E-04	2.00E-04
5.35E-01	9.78E+02	5.94E-03	6.78E-04	4.34E-03	5.85E-04	4.09E-03	6.26E-04	8.82E-04	1.84E-04
6.11E-01	9.85E+02	4.97E-03	8.54E-04	5.14E-03	3.53E-04	5.01E-03	7.00E-04	8.51E-04	1.53E-04
6.87E-01	9.98E+02	3.78E-03	1.15E-03	5.96E-03	1.77E-04	5.51E-03	7.67E-04	7.44E-04	9.74E-05
7.61E-01	1.01E+03	2.83E-03	1.46E-03	6.49E-03	9.52E-05	5.74E-03	7.78E-04	5.92E-04	6.16E-05
8.35E-01	1.01E+03	2.14E-03	1.81E-03	6.69E-03	4.74E-05	6.00E-03	7.42E-04	3.29E-04	3.94E-05
9.10E-01	1.02E+03	1.84E-03	1.97E-03	6.77E-03	4.74E-05	6.14E-03	6.83E-04	2.20E-04	2.95E-05

Table 13 VPFR Experimental data: 0.33% C₃H₆ 2.10% O₂ 97.57% N₂, $\phi=0.71$ $p=12.5$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
2.49E-02	8.42E+02	2.12E-02	5.39E-05	1.00E-04	3.12E-03	3.66E-04	3.66E-06	1.20E-05	2.01E-05
5.81E-02	8.44E+02	2.12E-02	6.43E-05	1.35E-04	3.12E-03	3.32E-04	3.66E-06	1.20E-05	2.52E-05
1.00E-01	8.43E+02	2.10E-02	7.78E-05	1.73E-04	3.06E-03	3.81E-04	3.66E-06	1.20E-05	3.08E-05
1.57E-01	8.43E+02	2.10E-02	8.64E-05	1.89E-04	3.09E-03	3.97E-04	3.66E-06	3.20E-05	3.42E-05
2.31E-01	8.42E+02	2.08E-02	1.14E-04	2.78E-04	3.01E-03	4.98E-04	3.66E-06	3.97E-05	5.26E-05
3.20E-01	8.46E+02	2.05E-02	1.48E-04	5.54E-04	2.81E-03	7.14E-04	3.66E-06	6.81E-05	8.37E-05
4.21E-01	8.52E+02	1.95E-02	2.13E-04	1.20E-03	2.34E-03	1.25E-03	6.61E-05	1.32E-04	1.37E-04
5.26E-01	8.68E+02	1.85E-02	3.29E-04	1.81E-03	1.95E-03	1.96E-03	1.55E-04	2.41E-04	1.63E-04
6.31E-01	8.79E+02	1.63E-02	5.96E-04	3.32E-03	1.20E-03	3.62E-03	2.01E-04	3.40E-04	1.46E-04
7.36E-01	8.98E+02	1.48E-02	8.52E-04	4.38E-03	8.18E-04	5.56E-03	2.90E-04	4.28E-04	1.28E-04
8.39E-01	9.17E+02	1.33E-02	1.32E-03	5.48E-03	4.33E-04	7.62E-03	4.25E-04	3.72E-04	8.65E-05
9.39E-01	9.31E+02	1.16E-02	1.92E-03	6.28E-03	1.35E-04	7.74E-03	4.39E-04	3.02E-04	5.07E-05
1.04E+00	9.42E+02	1.05E-02	2.63E-03	6.43E-03	2.50E-05	7.85E-03	3.82E-04	1.62E-04	4.22E-05

Table 14 VPFR Experimental data: 0.33% C₃H₆ 1.49% O₂ 98.18% N₂, $\phi=1.00$ $p=12.5$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
2.45E-02	8.58E+02	1.47E-02	6.16E-05	1.02E-04	3.18E-03	7.91E-04	3.66E-06	1.20E-05	2.23E-05
9.89E-02	8.63E+02	1.47E-02	7.36E-05	1.32E-04	3.21E-03	6.66E-04	3.66E-06	1.20E-05	2.57E-05
2.27E-01	8.58E+02	1.44E-02	1.27E-04	2.61E-04	3.11E-03	6.17E-04	3.66E-06	3.71E-05	3.97E-05
4.16E-01	8.61E+02	1.44E-02	1.23E-04	3.27E-04	3.02E-03	6.13E-04	3.66E-06	5.30E-05	6.60E-05
6.29E-01	8.60E+02	1.41E-02	1.51E-04	5.14E-04	2.81E-03	7.46E-04	4.14E-05	8.43E-05	1.01E-04
7.36E-01	8.61E+02	1.37E-02	1.78E-04	8.21E-04	2.57E-03	9.64E-04	8.75E-05	1.83E-04	1.29E-04
8.44E-01	8.69E+02	1.27E-02	2.54E-04	1.58E-03	2.14E-03	1.56E-03	1.83E-04	3.42E-04	1.68E-04
9.48E-01	9.10E+02	8.93E-03	8.38E-04	4.57E-03	9.10E-04	3.84E-03	3.86E-04	5.64E-04	1.61E-04
1.05E+00	9.45E+02	5.48E-03	1.82E-03	6.59E-03	1.65E-04	5.07E-03	5.05E-04	3.91E-04	8.12E-05
1.24E+00	9.55E+02	4.24E-03	2.47E-03	6.85E-03	1.75E-05	7.47E-03	5.24E-04	2.81E-04	2.62E-05
1.34E+00	9.54E+02	3.98E-03	2.66E-03	6.84E-03	1.53E-05	7.74E-03	4.92E-04	1.94E-04	2.03E-05
1.54E+00	9.56E+02	3.65E-03	3.01E-03	6.65E-03	8.20E-06	7.88E-03	4.17E-04	1.36E-04	1.87E-05
1.64E+00	9.64E+02	3.51E-03	3.34E-03	6.69E-03	6.50E-06	7.96E-03	3.82E-04	6.99E-05	1.64E-05

Table 15 VPFR Experimental data: 0.33% C₃H₆ 1.15% O₂ 98.52% N₂, $\phi=1.29$ $p=12.5$ atm.

Mole Fraction									
Time, s	T, K	O ₂	CO ₂	CO	C ₃ H ₆	H ₂ O	CH ₄	C ₂ H ₄	CH ₂ O
2.41E-02	8.80E+02	1.13E-02	5.25E-05	8.63E-05	3.18E-03	3.05E-04	3.66E-06	1.20E-05	1.80E-05
9.72E-02	8.79E+02	1.12E-02	6.44E-05	1.12E-04	3.21E-03	3.09E-04	3.66E-06	1.20E-05	2.19E-05
2.24E-01	8.75E+02	1.10E-02	9.56E-05	2.06E-04	3.16E-03	4.20E-04	3.66E-06	3.38E-05	3.50E-05
4.09E-01	8.78E+02	1.08E-02	1.21E-04	3.01E-04	3.03E-03	5.57E-04	3.66E-06	5.92E-05	5.41E-05
6.19E-01	8.75E+02	1.07E-02	1.29E-04	3.37E-04	2.99E-03	6.15E-04	3.66E-06	6.73E-05	6.63E-05
7.25E-01	8.74E+02	1.06E-02	1.33E-04	3.83E-04	2.89E-03	6.56E-04	6.16E-05	1.16E-04	7.94E-05
8.32E-01	8.75E+02	1.05E-02	1.39E-04	5.06E-04	2.73E-03	7.76E-04	6.03E-05	1.87E-04	1.06E-04
9.38E-01	8.85E+02	9.71E-03	1.65E-04	1.03E-03	2.32E-03	1.13E-03	1.44E-04	3.97E-04	1.57E-04
1.04E+00	9.14E+02	7.44E-03	3.72E-04	3.00E-03	1.41E-03	2.86E-03	4.57E-04	6.31E-04	2.01E-04
1.14E+00	9.33E+02	4.39E-03	8.00E-04	5.46E-03	4.09E-04	4.65E-03	6.12E-04	7.43E-04	1.17E-04
1.24E+00	9.44E+02	3.21E-03	1.11E-03	6.33E-03	1.91E-04	5.93E-03	7.04E-04	7.74E-04	8.72E-05
1.34E+00	9.57E+02	2.94E-03	1.33E-03	6.52E-03	1.16E-04	6.19E-03	7.11E-04	6.04E-04	6.79E-05
1.44E+00	9.60E+02	2.38E-03	1.53E-03	6.84E-03	6.41E-05	6.22E-03	7.16E-04	4.90E-04	5.38E-05

High Pressure Laminar Flow Reactor data

Table 16 HPLFR Experimental data: 0.40% C₃H₆ 5.14% O₂ 94.45% N₂, $\phi=0.35$ p=15 atm, 800 K.

PPM					T Profile	
Time, s	O ₂	C ₃ H ₆	CO	CO ₂	Time, s	T, K
3.67E-01	5.19E+04	3.99E+03			1.22E-01	802
4.90E-01	5.17E+04	3.99E+03			2.45E-01	806
6.12E-01	5.18E+04	3.94E+03			3.67E-01	808
7.35E-01	5.17E+04	3.98E+03			4.90E-01	807
8.57E-01	5.18E+04	3.93E+03			6.12E-01	806
9.79E-01	5.18E+04	3.88E+03			7.35E-01	803
1.10E+00	5.17E+04	3.85E+03			8.57E-01	802
1.22E+00	5.18E+04	3.78E+03			9.79E-01	800
1.35E+00	5.13E+04	3.71E+03			1.10E+00	800
1.47E+00	5.13E+04	3.56E+03		1.02E+01	1.22E+00	800
1.59E+00	5.08E+04	3.35E+03	1.90E+02	2.84E+01	1.35E+00	802
1.71E+00	5.00E+04	3.07E+03	4.56E+02	4.98E+01	1.47E+00	804
1.84E+00	4.91E+04	2.57E+03	9.89E+02	8.41E+01	1.59E+00	807
					1.71E+00	810
					1.84E+00	813
					1.96E+00	815
					2.08E+00	816
					2.20E+00	815
					2.45E+00	808

Table 17 HPLFR Experimental data: 0.45% C₃H₆ 4.05% O₂ 95.50% N₂, $\phi=0.50$, $p=15$ atm, 800 K.

PPM					T Profile	
Time, s	O ₂	C ₃ H ₆	CO	CO ₂	Time, s	T, K
3.67E-01	4.07E+04	4.51E+03			1.22E-01	802
4.90E-01	4.06E+04	4.52E+03			2.45E-01	805
6.12E-01	4.06E+04	4.49E+03			3.67E-01	806
7.35E-01	4.07E+04	4.47E+03			4.90E-01	806
8.57E-01	4.07E+04	4.44E+03			6.12E-01	804
9.79E-01	4.06E+04	4.46E+03			7.35E-01	802
1.10E+00	4.07E+04	4.39E+03			8.57E-01	800
1.22E+00	4.03E+04	4.42E+03			9.79E-01	799
1.35E+00	4.04E+04	4.35E+03			1.10E+00	799
1.47E+00	4.01E+04	4.28E+03			1.22E+00	799
1.59E+00	3.99E+04	4.20E+03			1.35E+00	800
1.71E+00	3.99E+04	4.07E+03			1.47E+00	802
1.84E+00	3.94E+04	3.85E+03	1.14E+02	2.52E+01	1.59E+00	804
					1.71E+00	808
					1.84E+00	811
					1.96E+00	815
					2.08E+00	818
					2.20E+00	820
					2.33E+00	818
					2.45E+00	817

Table 18 HPLFR Experimental data: 0.50% C₃H₆ 2.50% O₂ 97.25% N₂, $\phi=1.0$, $p=15$ atm, 800 K.

PPM						T Profile	
Time, s	O ₂	C ₃ H ₆	CO	CO ₂	H ₂ O	Time, s	T, K
4.90E-01	2.25E+04	4.98E+03				2.45E-01	804
7.35E-01	2.26E+04	5.01E+03				4.90E-01	804
9.80E-01	2.26E+04	5.00E+03				7.35E-01	802
1.22E+00	2.26E+04	5.01E+03				9.80E-01	800
1.47E+00	2.25E+04	4.95E+03				1.22E+00	800
1.71E+00	2.25E+04	4.92E+03				1.47E+00	801
1.96E+00	2.24E+04	4.84E+03			1.15E+02	1.71E+00	802
2.20E+00	2.23E+04	4.73E+03	0.00E+00	5.36E+00	1.63E+02	1.96E+00	803
2.45E+00	2.22E+04	4.65E+03	1.45E+02	1.07E+01	2.50E+02	2.20E+00	802
						2.45E+00	797

Table 19 HPLFR Experimental data: 0.62% C₃H₆ 2.25% O₂ 91.13% N₂, $\phi=1.25$, $p=15$ atm, 800 K.

PPM						T Profile	
Time, s	O ₂	C ₃ H ₆	CO	CO ₂	H ₂ O	Time, s	T, K
4.90E-01	2.26E+04	6.32E+03				2.45E-01	805
7.35E-01	2.25E+04	6.27E+03				4.90E-01	805
9.80E-01	2.25E+04	6.27E+03				7.35E-01	803
1.22E+00	2.25E+04	6.27E+03				9.80E-01	800
1.47E+00	2.25E+04	6.20E+03				1.22E+00	799
1.71E+00	2.24E+04	6.16E+03				1.47E+00	799
1.96E+00	2.23E+04	6.09E+03			1.38E+02	1.71E+00	798
2.08E+00	2.22E+04	6.05E+03		3.22E+00	1.59E+02	1.84E+00	798
2.20E+00	2.22E+04	6.00E+03		6.97E+00	1.76E+02	1.96E+00	798
2.33E+00	2.21E+04	5.92E+03		1.13E+01	2.39E+02	2.08E+00	798
2.45E+00	2.20E+04	5.82E+03	1.09E+02	1.45E+01	2.99E+02	2.20E+00	797
						2.45E+00	794

Princeton Variable pressure flow reactor additional plots

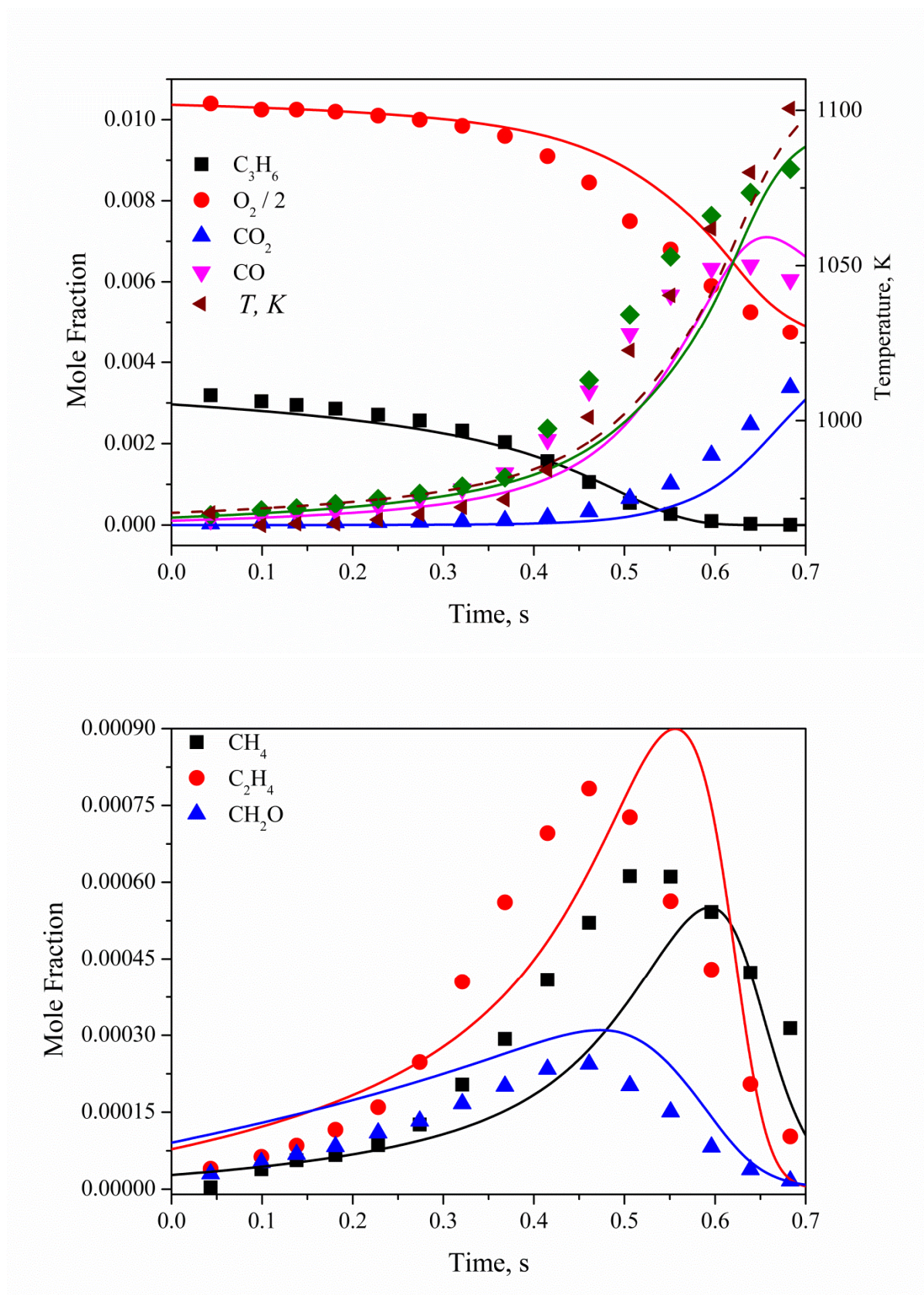


Figure 1: VPFR: 0.33% C_3H_6 2.10% O_2 97.57% N_2 , $\phi=0.71$, $p=6$ atm, time shift: -0.32s

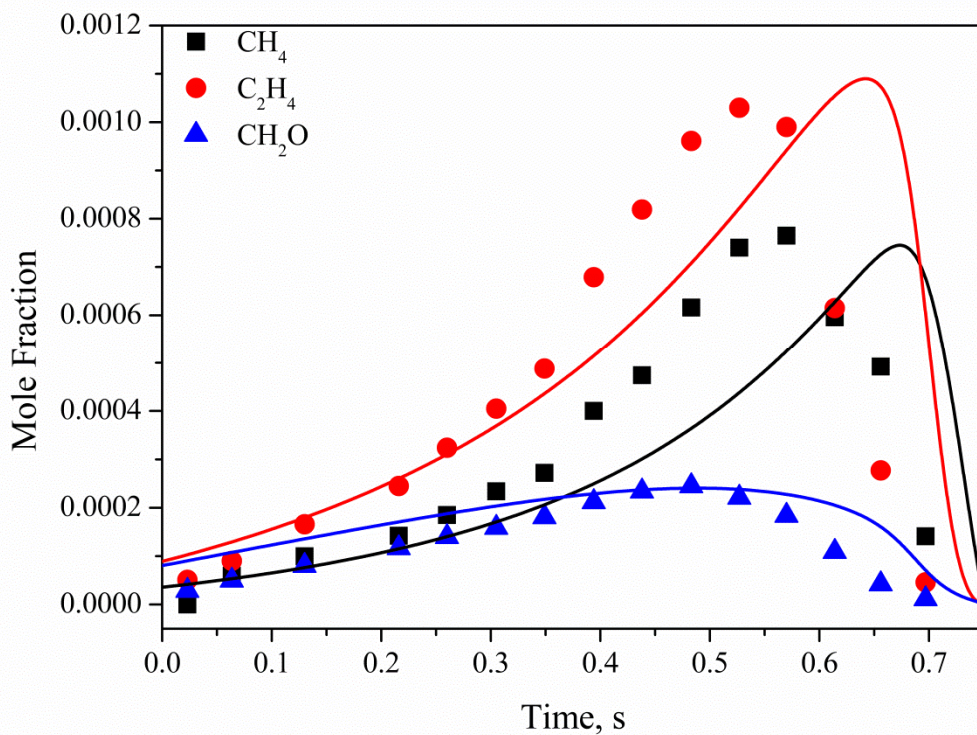
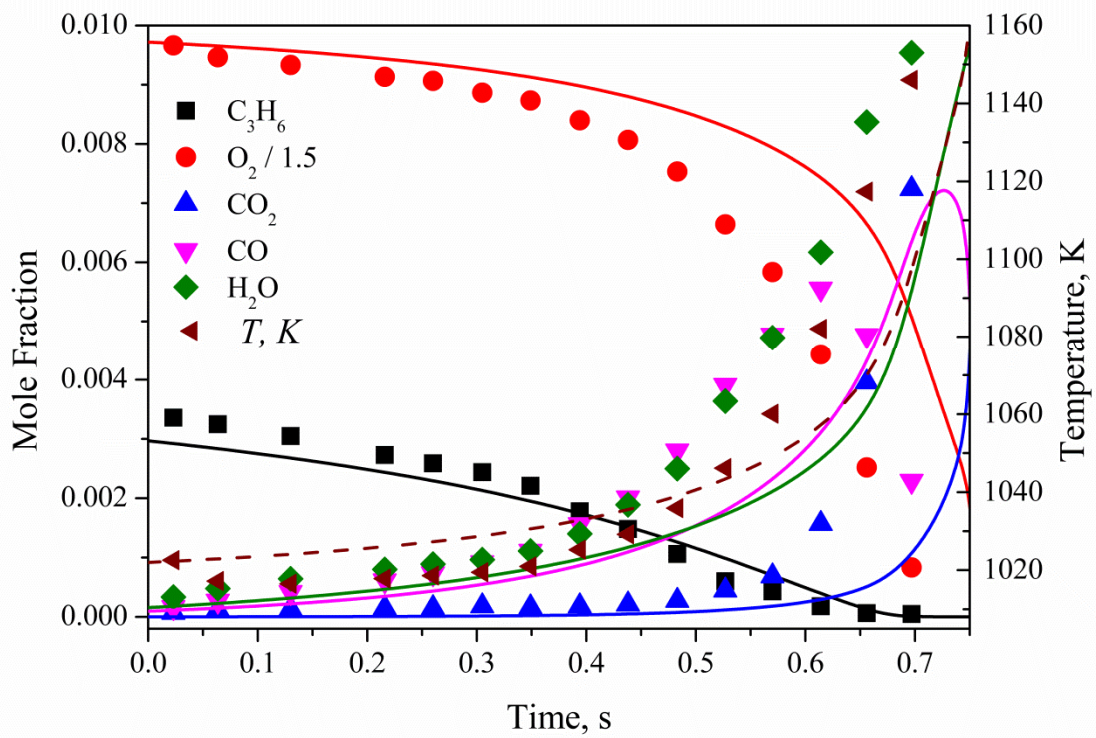


Figure 2: VPFR: 0.33% C_3H_6 1.48% O_2 98.19% N_2 , $\phi=1.00$, $p=6$ atm, time shift: -0.20s.

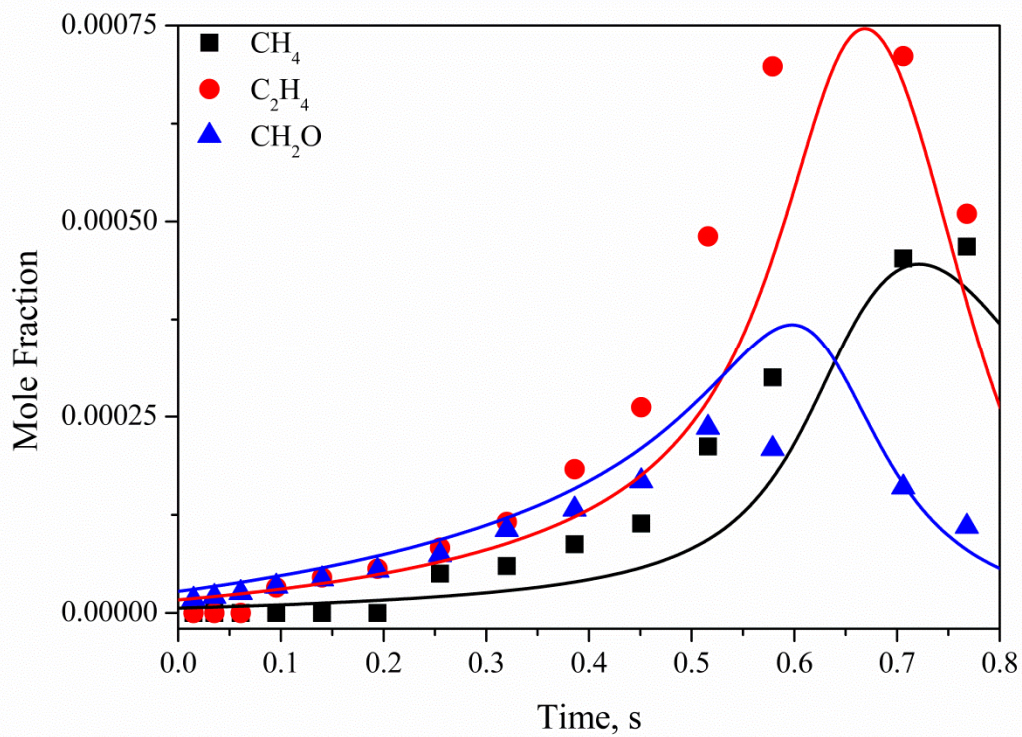
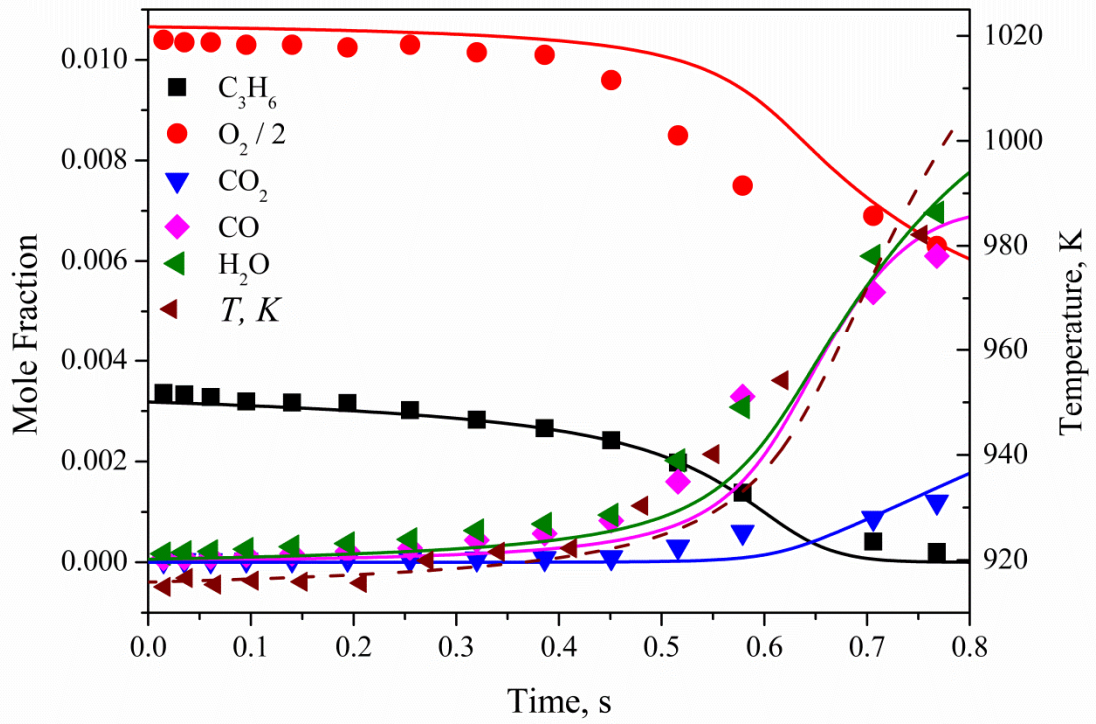


Figure 3: VPFR: 0.33% C_3H_6 2.14% O_2 97.53% N_2 , $\phi=0.71$, $p=8$ atm, time shift: -0.26s.

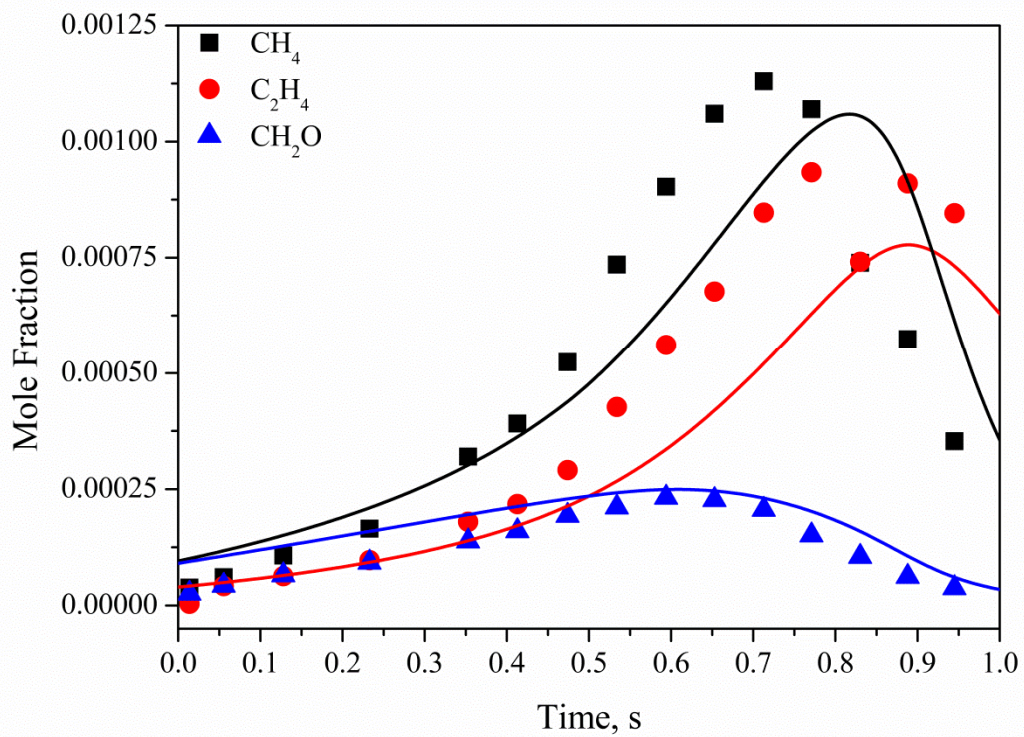
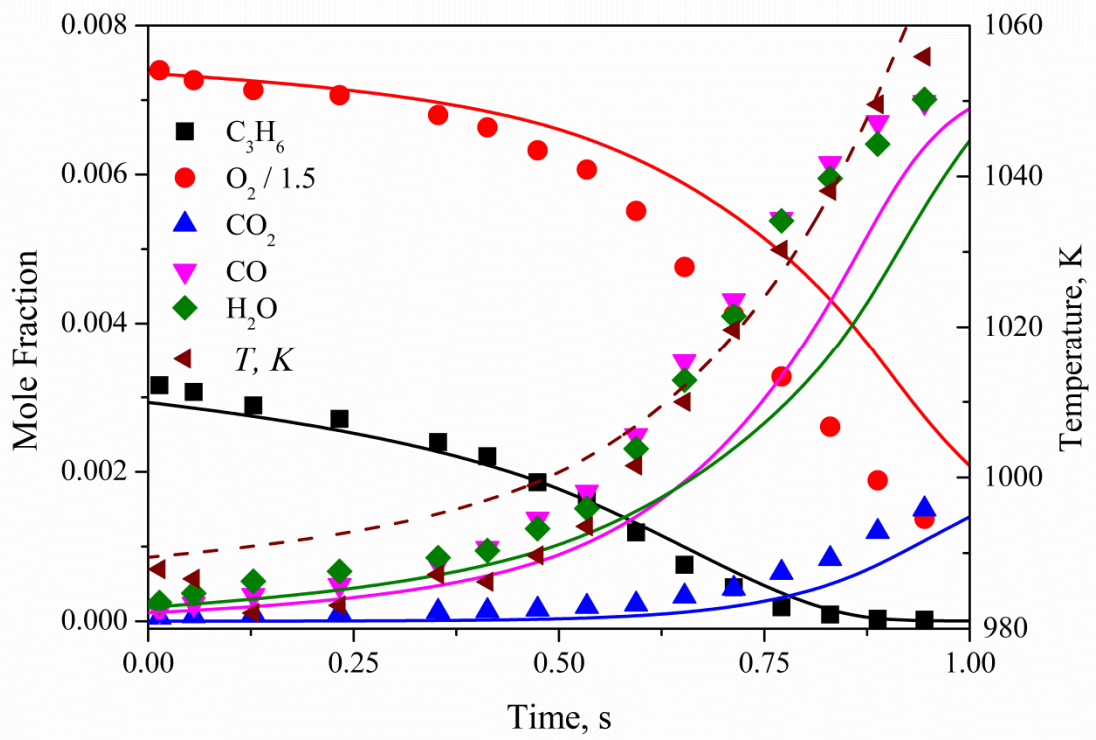


Figure 4: VPFR: 0.33% C_3H_6 1.13% O_2 98.54% N_2 , $\phi=1.31$ $p=8$ atm, time shift: -0.37s.

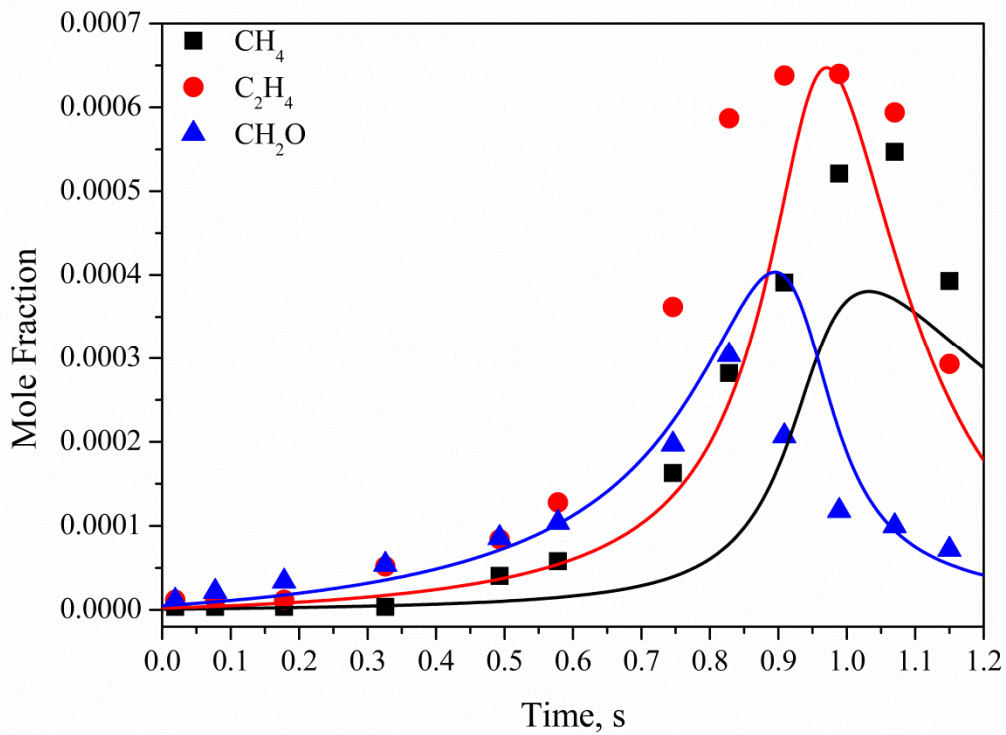
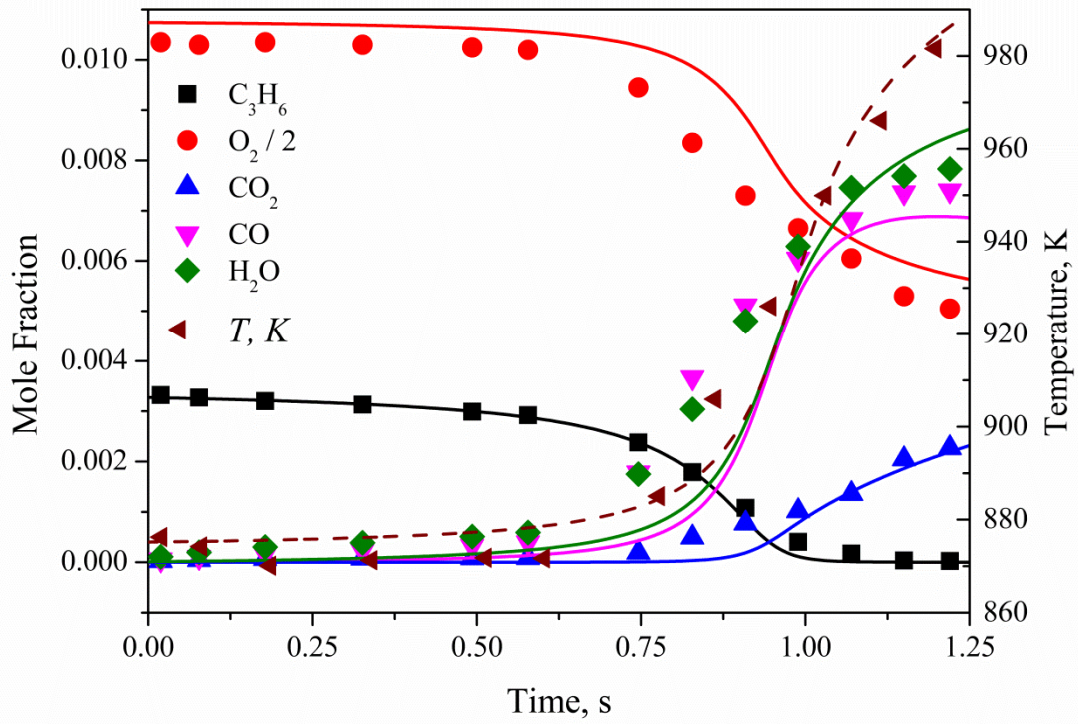


Figure 5: VPFR: 0.33% C_3H_6 2.14% O_2 97.53% N_2 , $\phi=0.70$ $p=10$ atm, time shift: -0.15s.

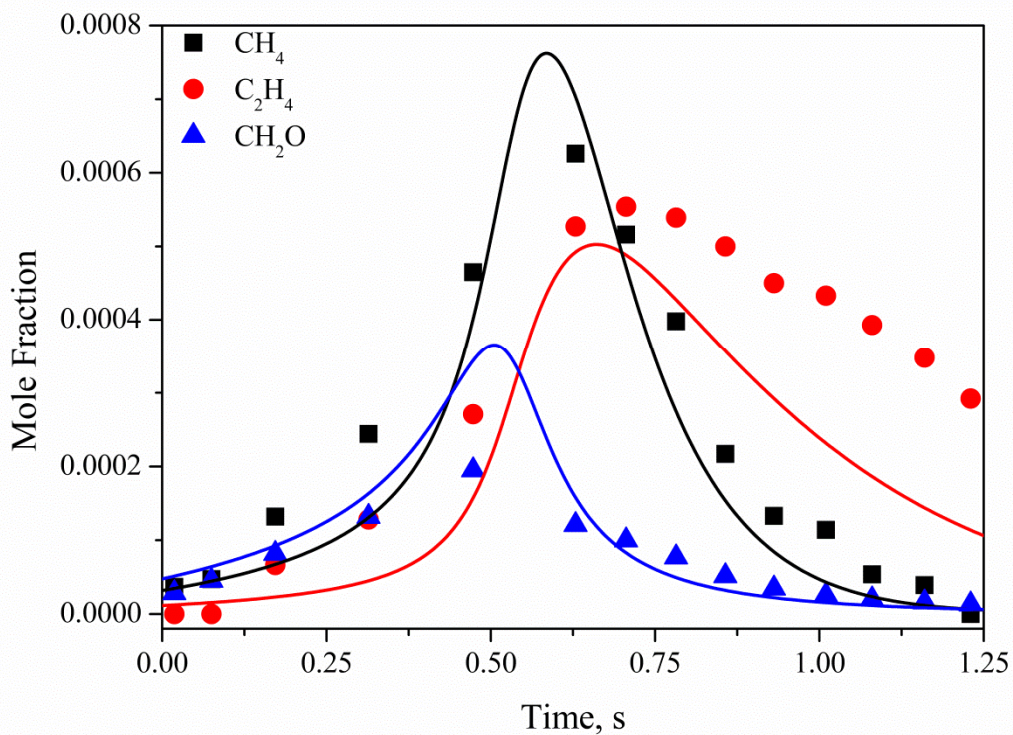
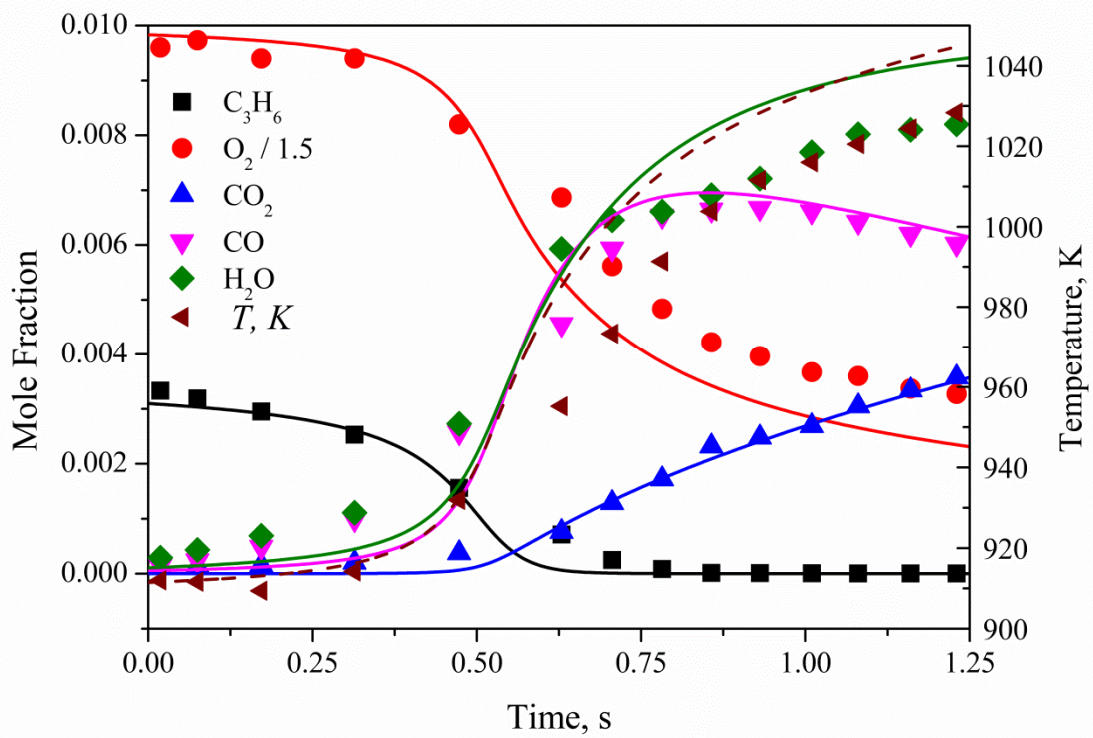


Figure 6: VPFR: 0.33% C₃H₆ 1.49% O₂ 98.18% N₂, $\phi=1.00$ p=10 atm, time shift: -0.45s.

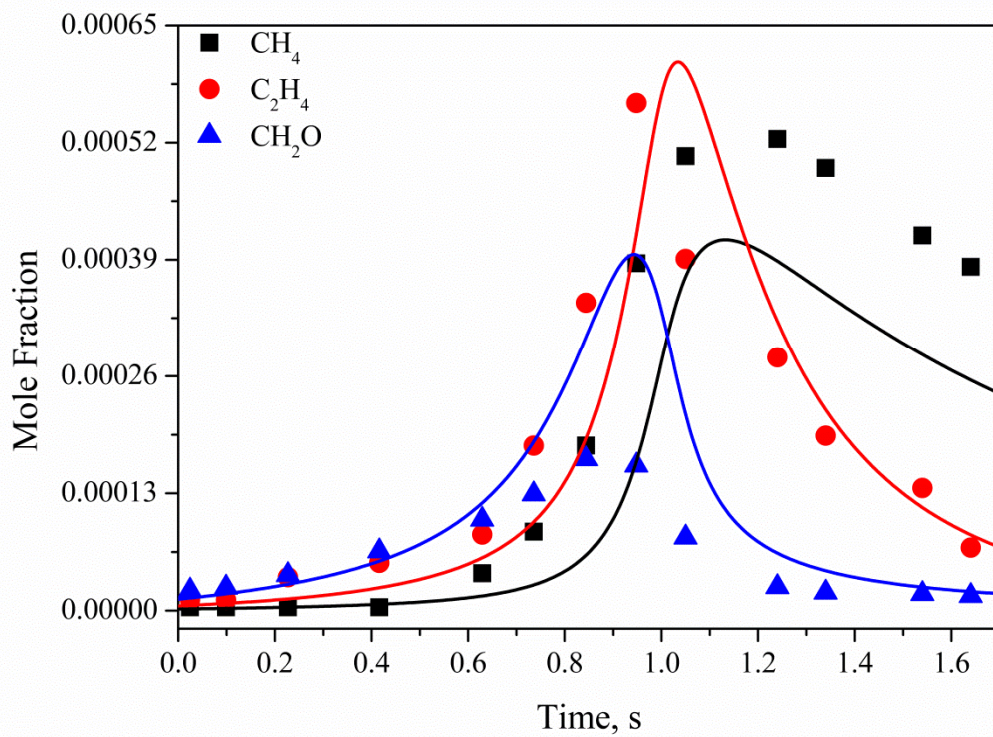
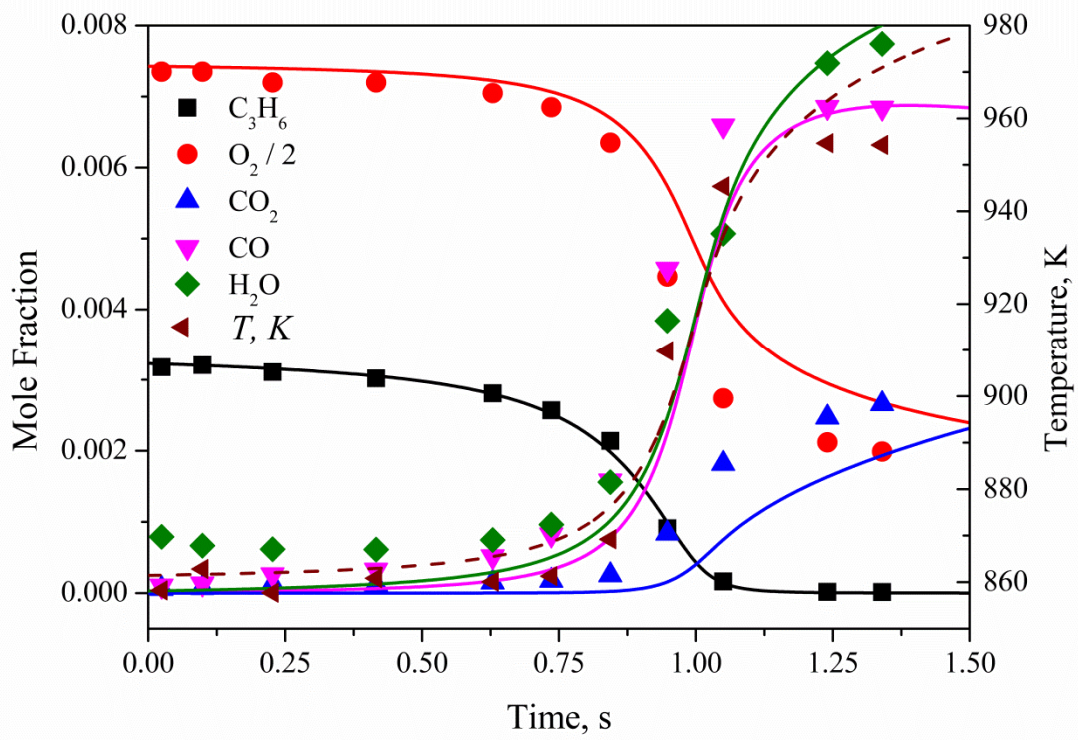


Figure 7: VPFR: 0.33% C_3H_6 1.49% O_2 98.18% N_2 , $\phi=1.00$ $p=12.5$ atm, time shift: -0.42s.

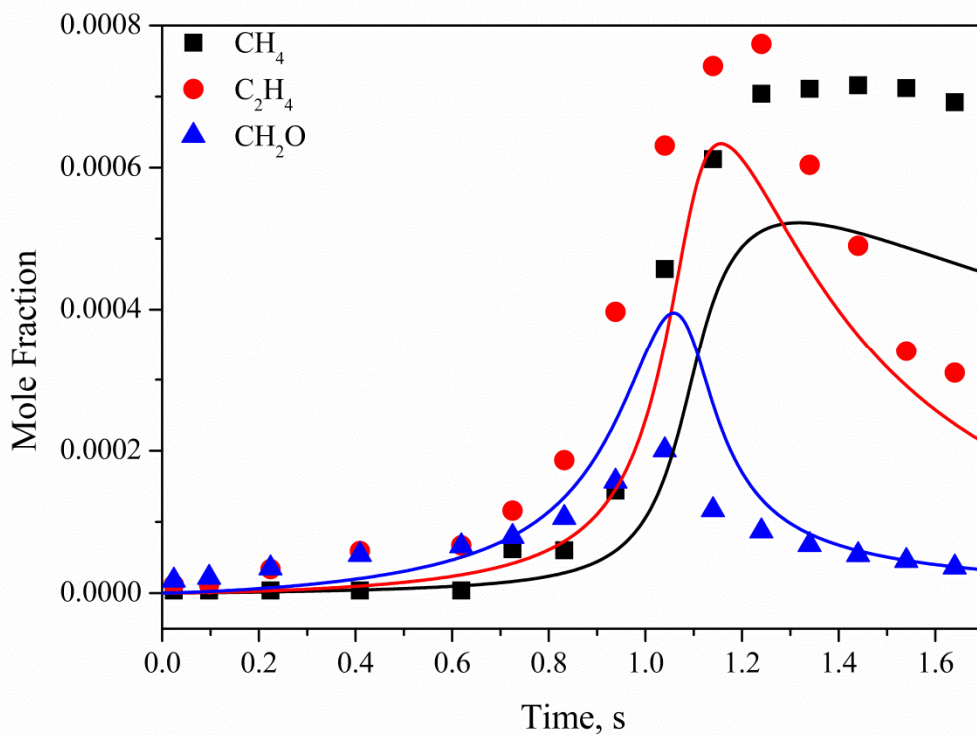
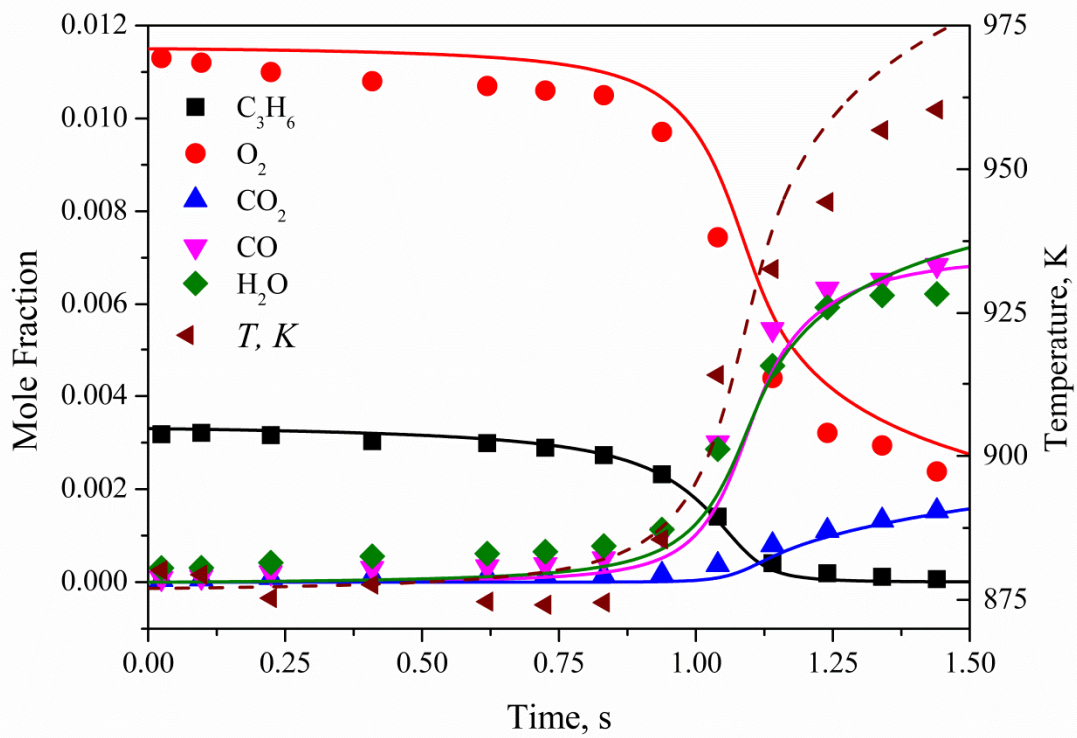


Figure 8: VPFR: 0.33% C_3H_6 1.15% O_2 98.52% N_2 , $\phi=1.29$ $p=12.5$ atm, time shift: -0.01s.

Mechanism validation

The mechanism presented in this study and other mechanisms [1–3] from the literature are compared with selected experimental data from the literature [3,7].

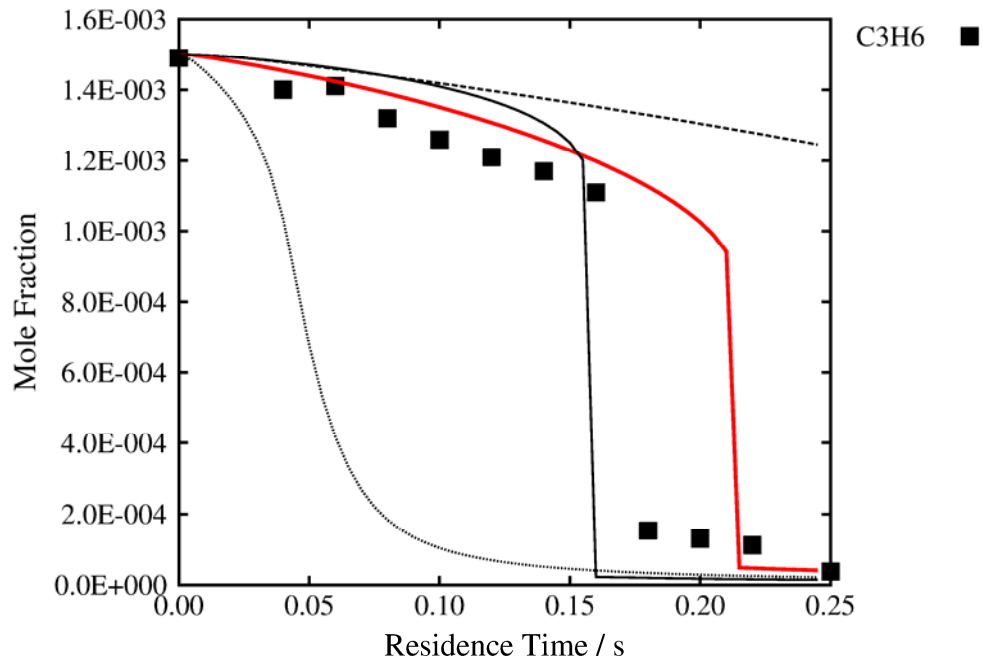
Throughout the supplementary material symbols represent experimental data and lines represent model predictions. The lines are set out as follows: — AramcoMech 2.0 as presented in this work, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], · · · USC II[3]. Not all of these mechanisms are validated against all of the conditions studied and are **included for comparative purposes**.

Literature data

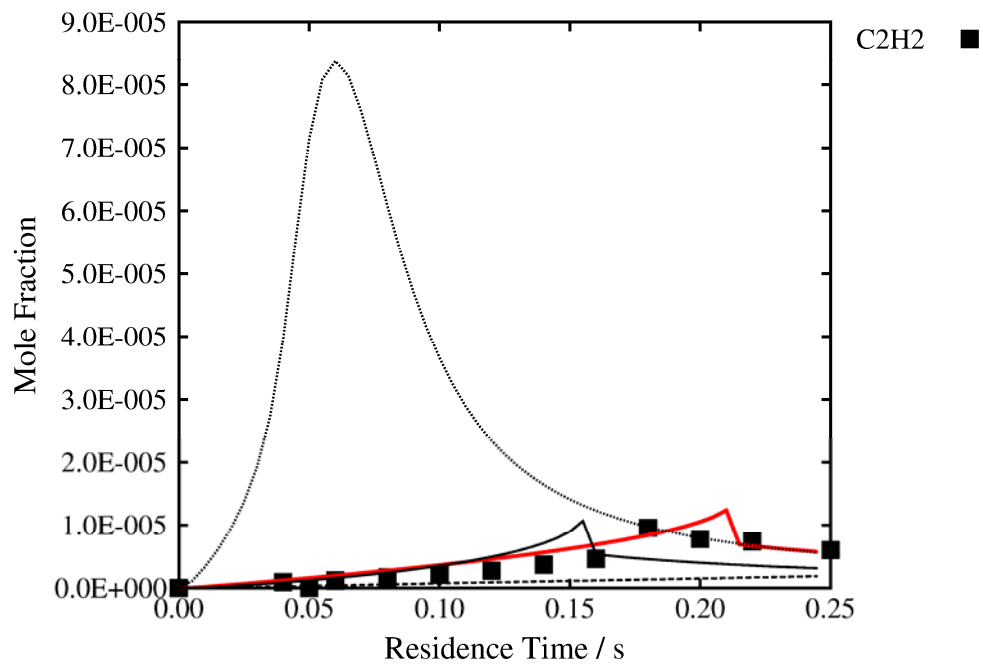
Jet-stirred reactor

Dagaut et al.[4]

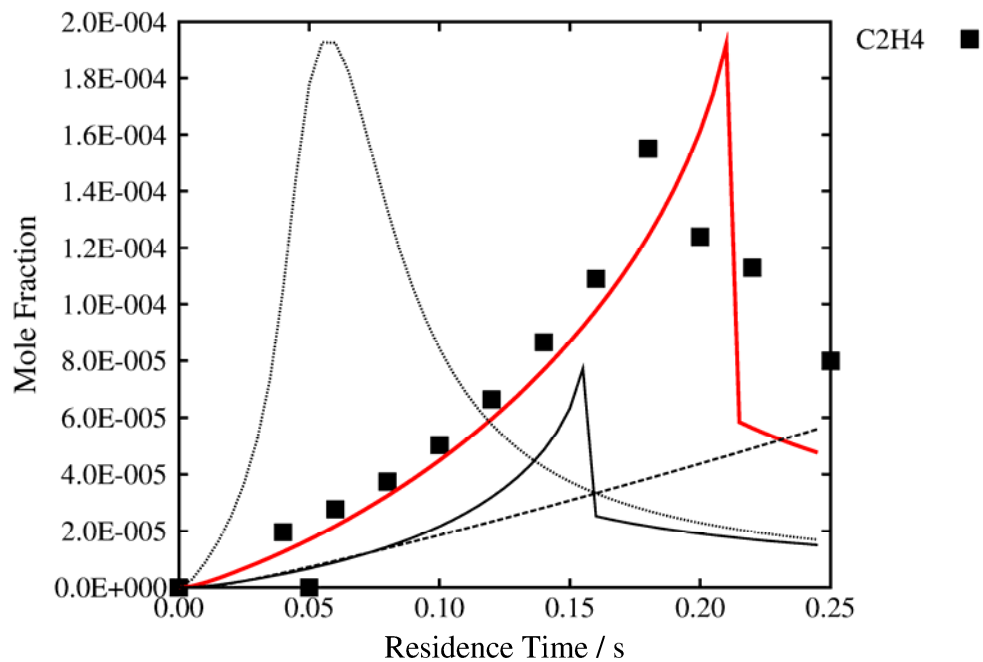
0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



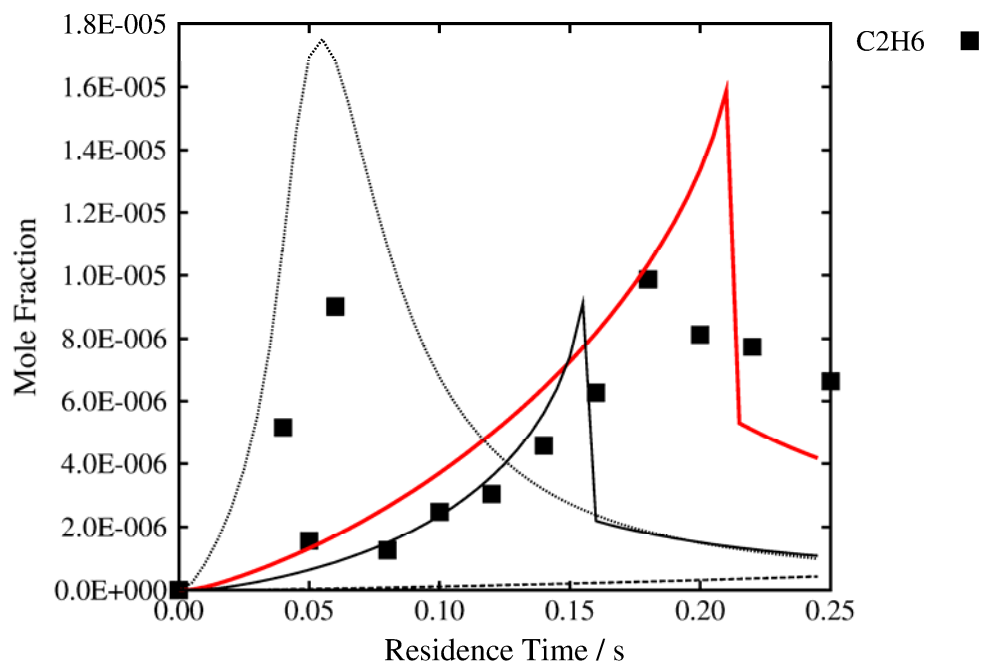
0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



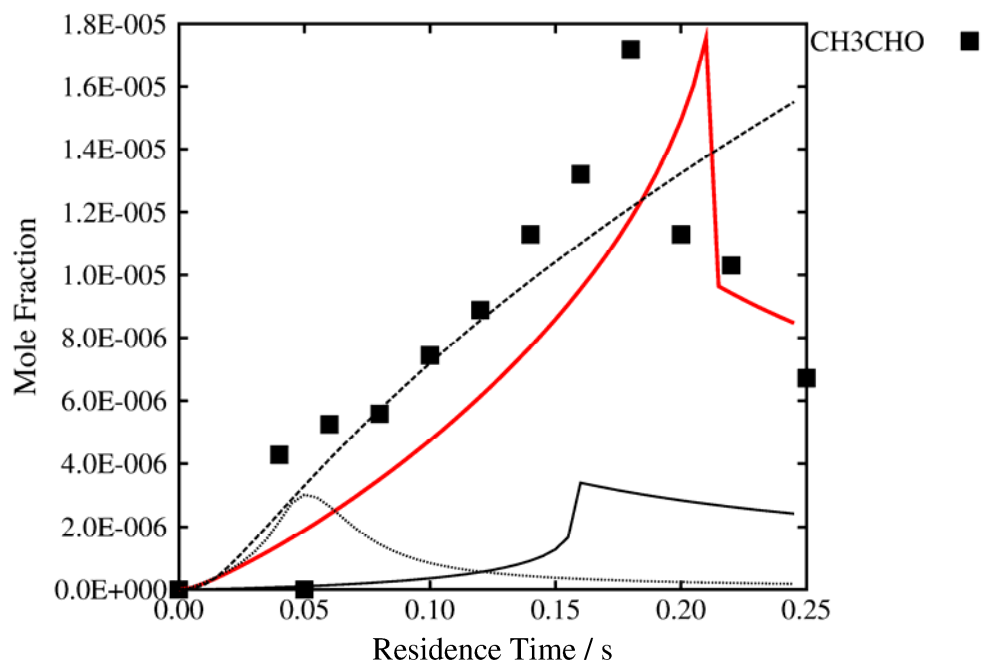
0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



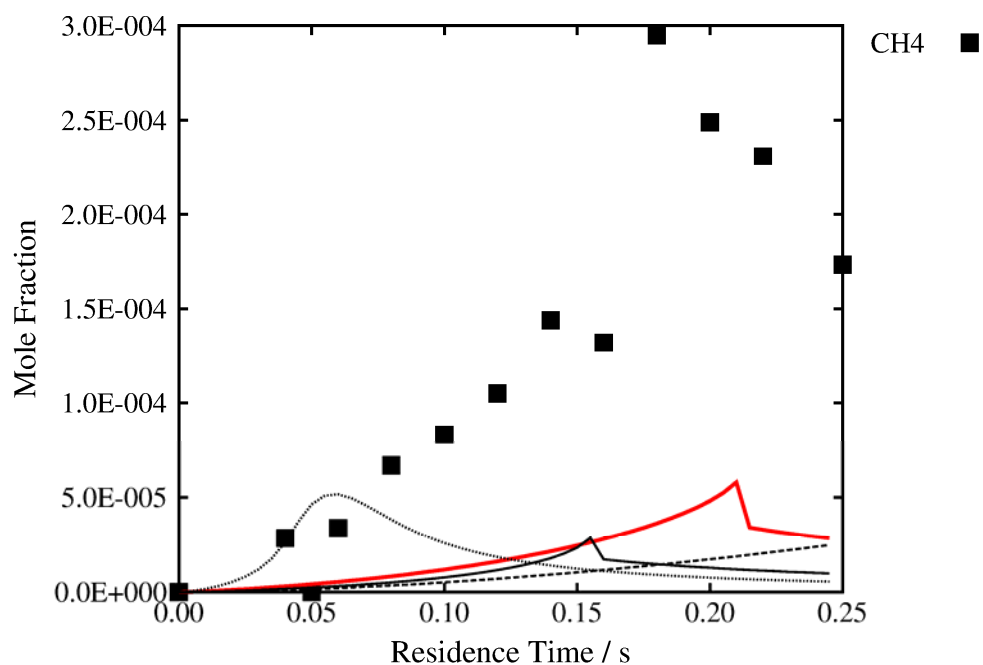
0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



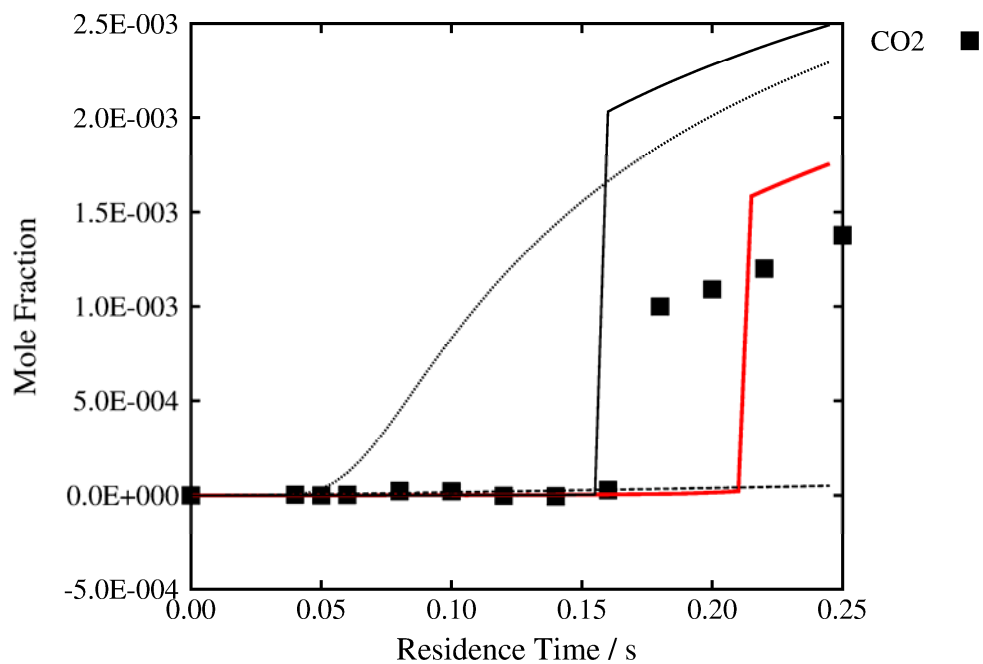
0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K



0.15% C₃H₆, 4.50% O₂ in N₂, $\Phi = 0.15$, $p = 1.0$ atm, $T = 1070$ K

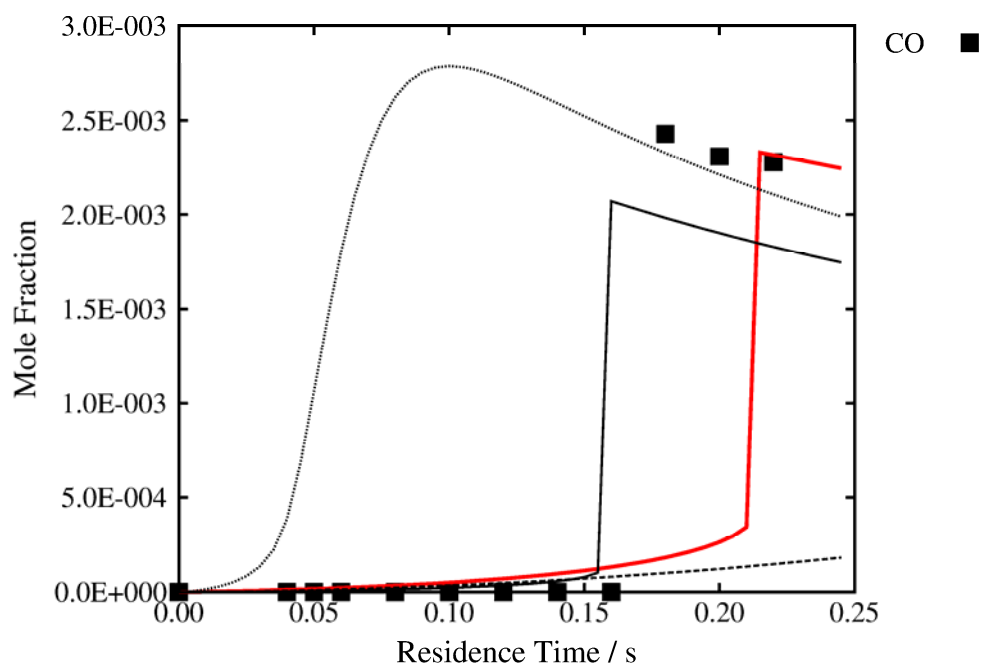
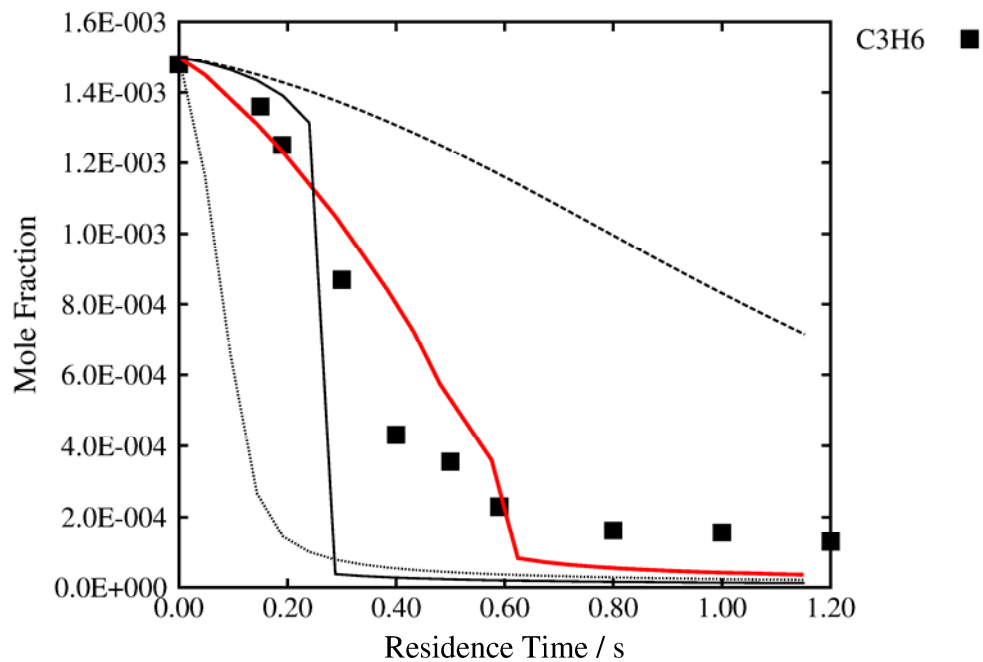
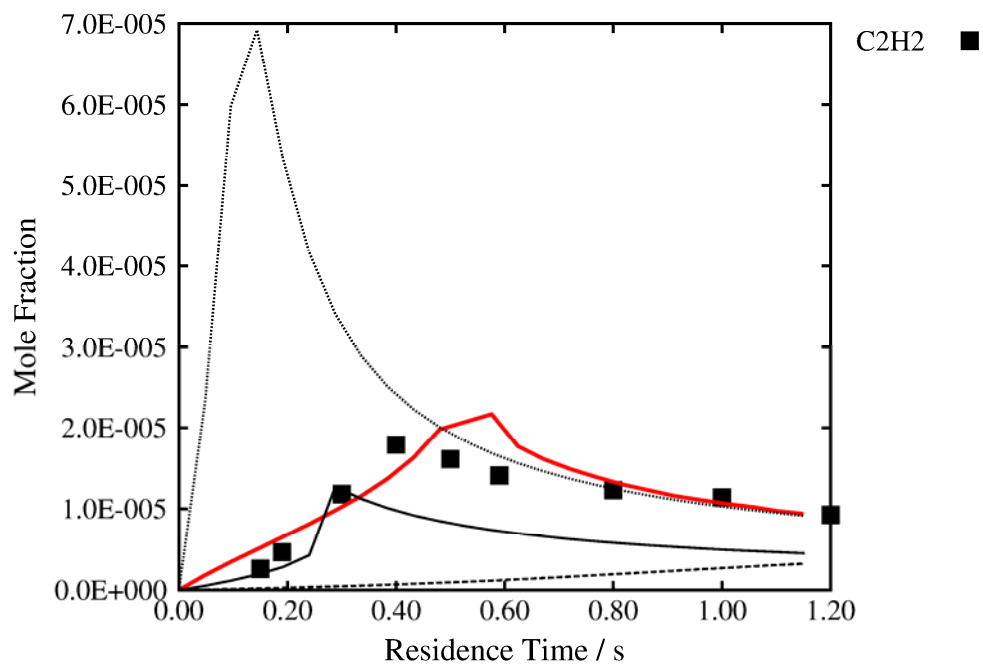


Figure 9 Jet-stirred reactor of propene/O₂/N₂. Symbols are experimental data [4] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], · · · USC II[3].

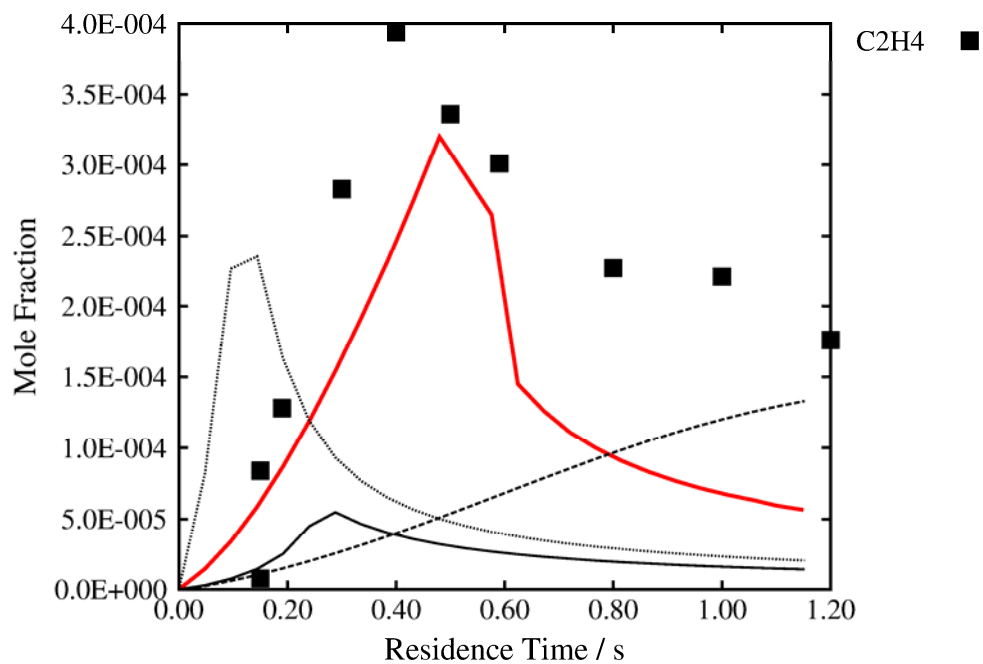
0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



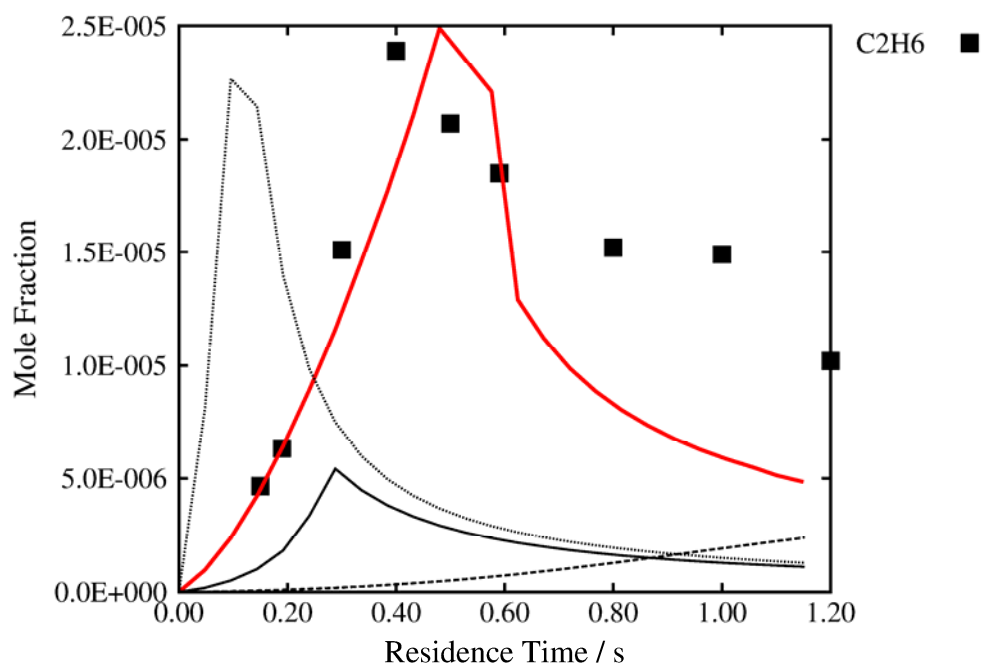
0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



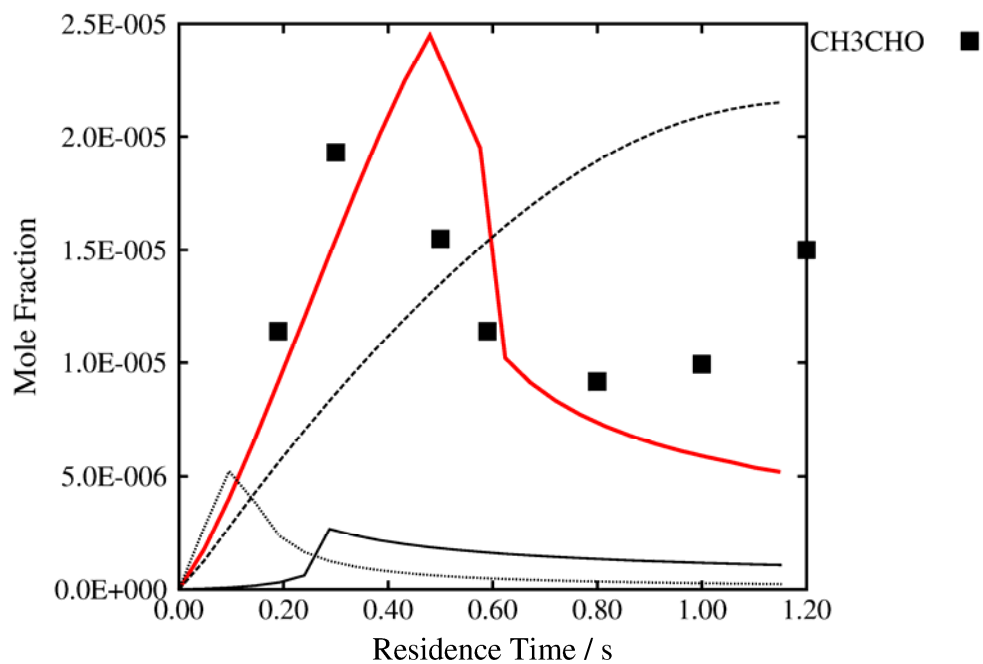
0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



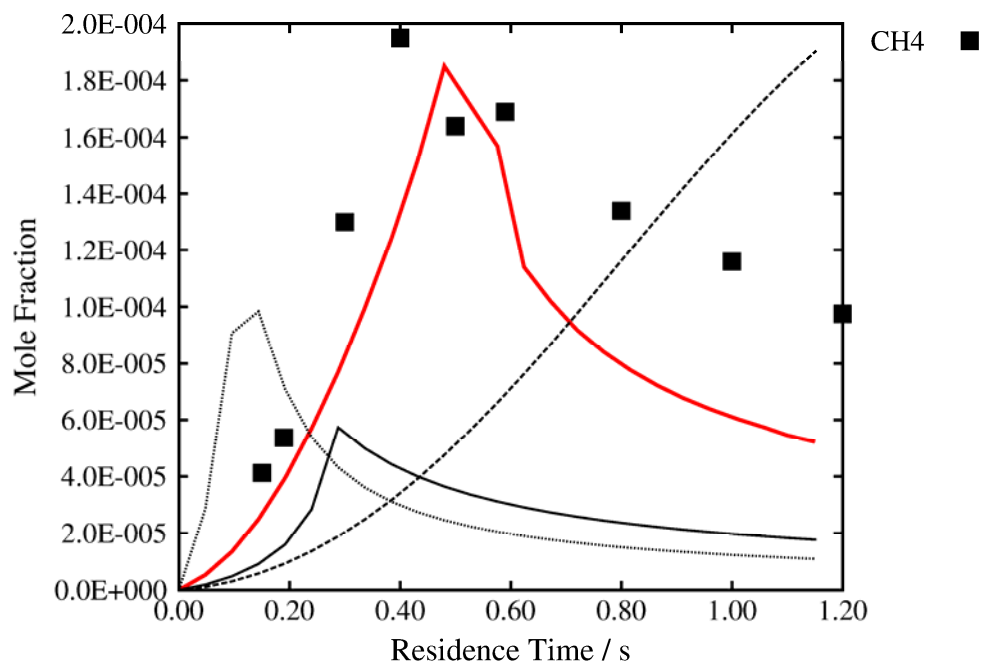
0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K



0.15% C₃H₆, 1.35% O₂ in N₂, $\Phi = 0.50$, $p = 5.0$ atm, $T = 1050$ K

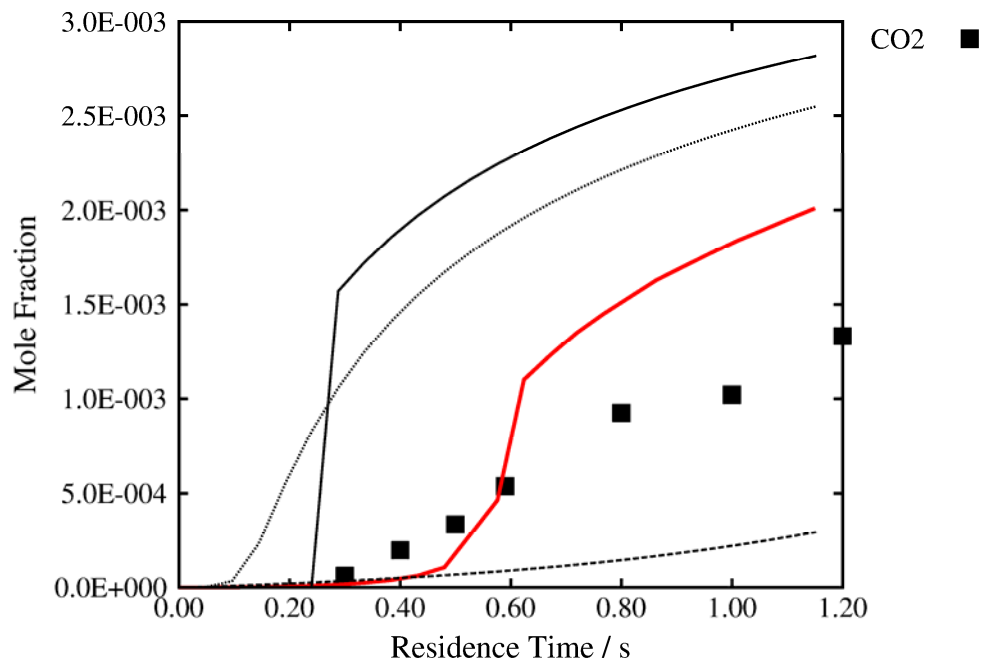
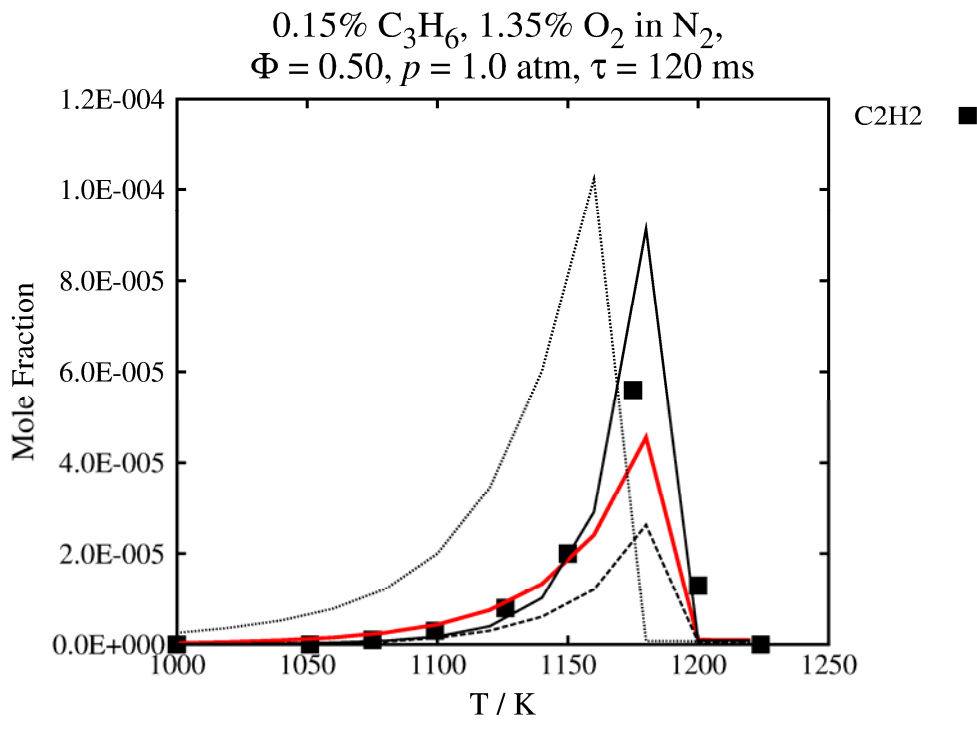
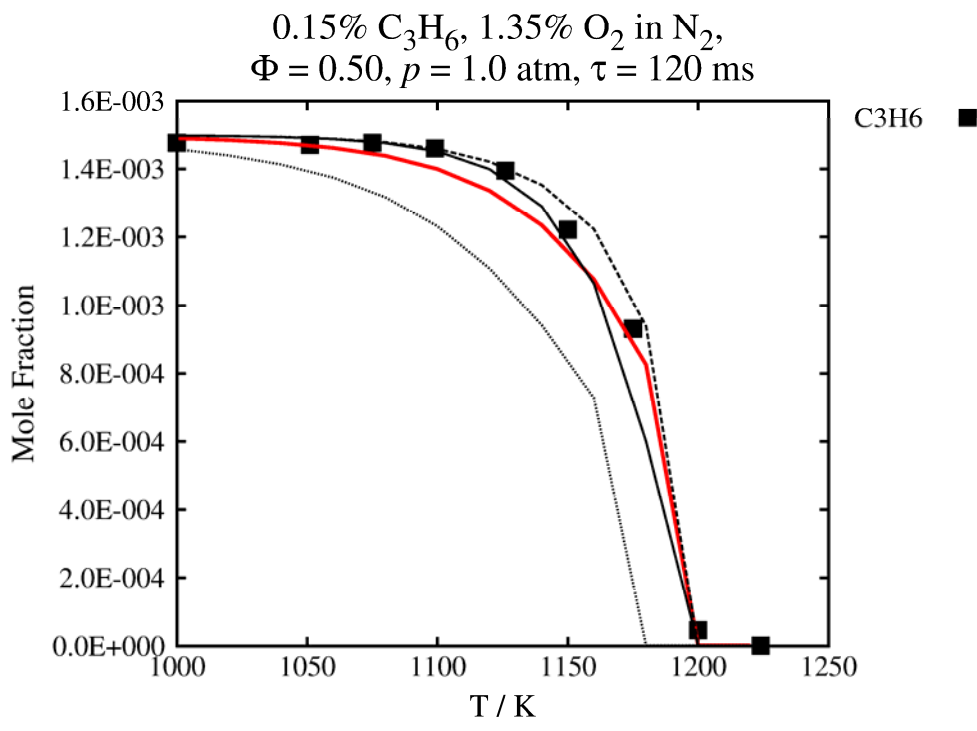
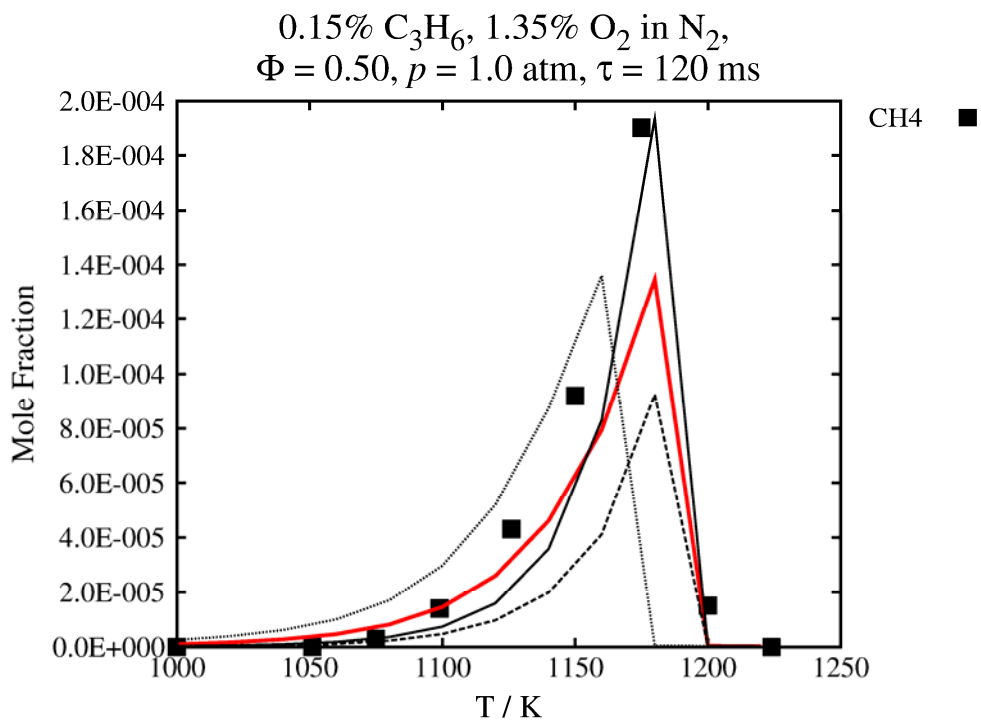
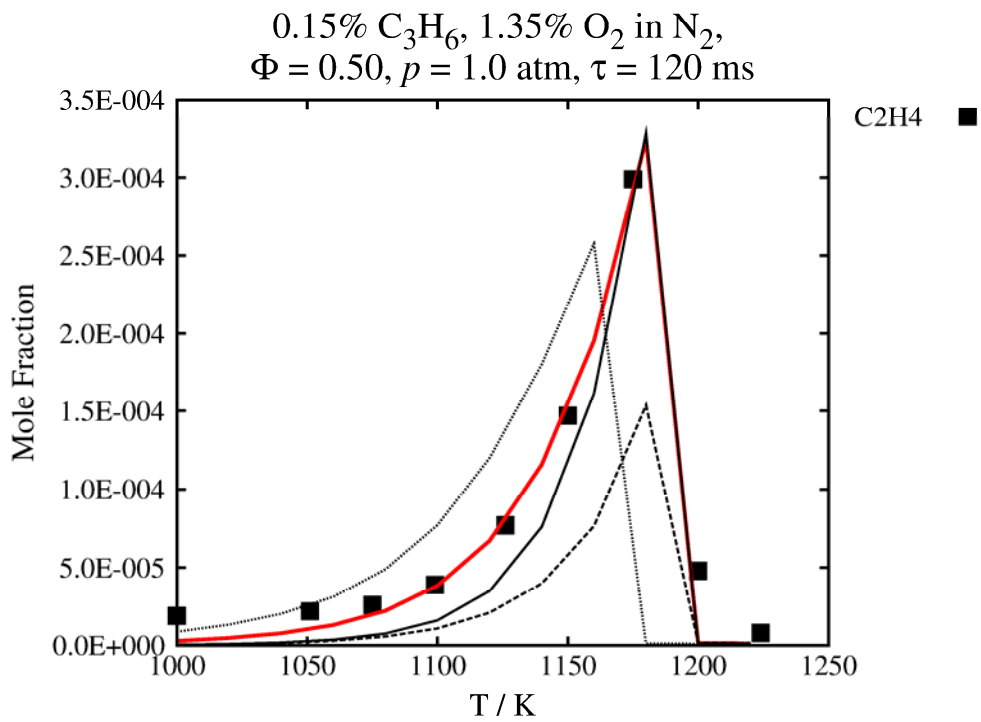
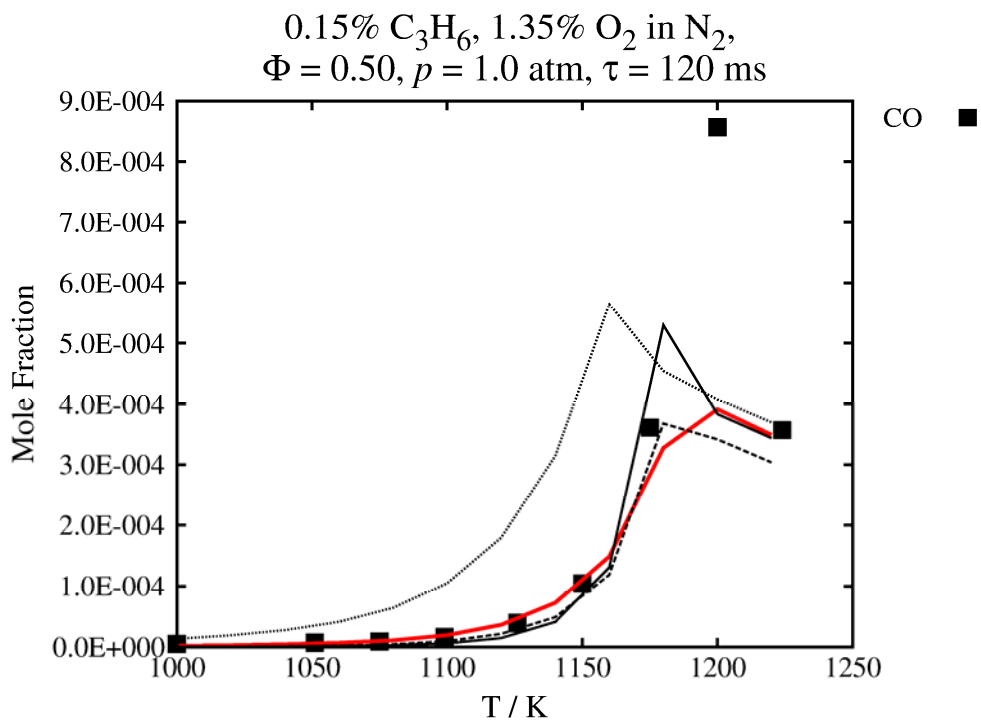
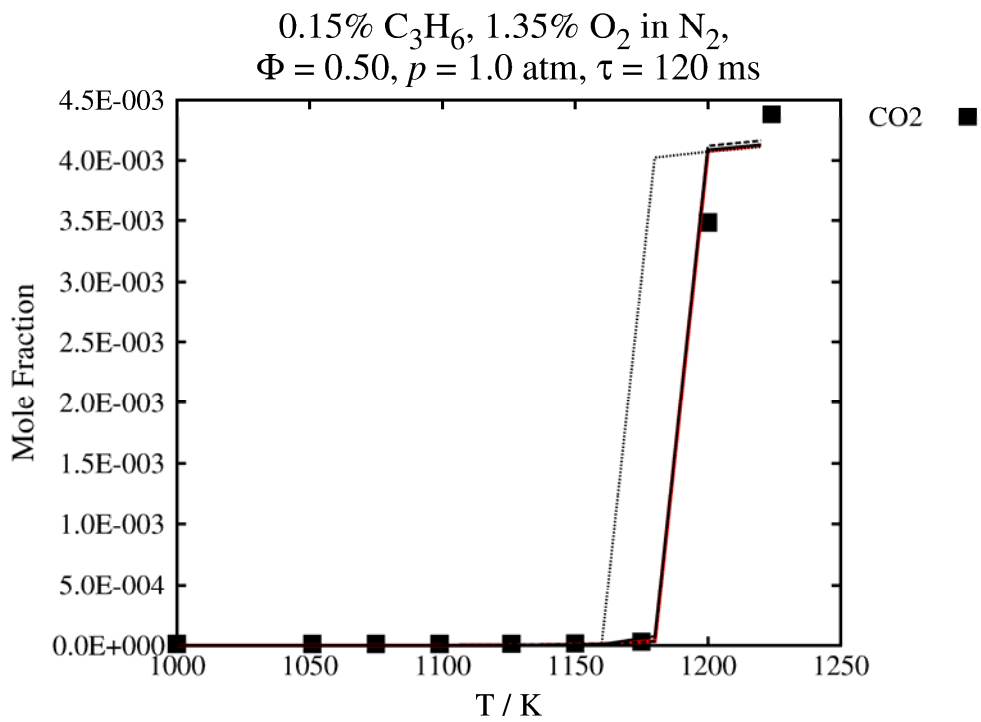


Figure 10 Jet-stirred reactor of propene/O₂/N₂. Symbols are experimental data [4] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].







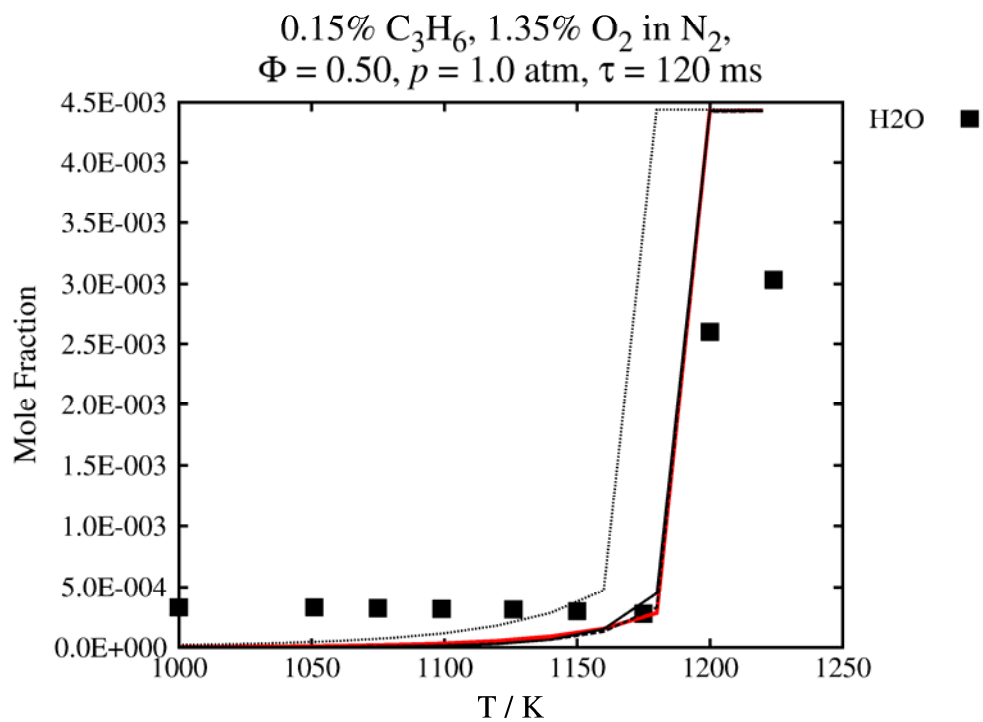
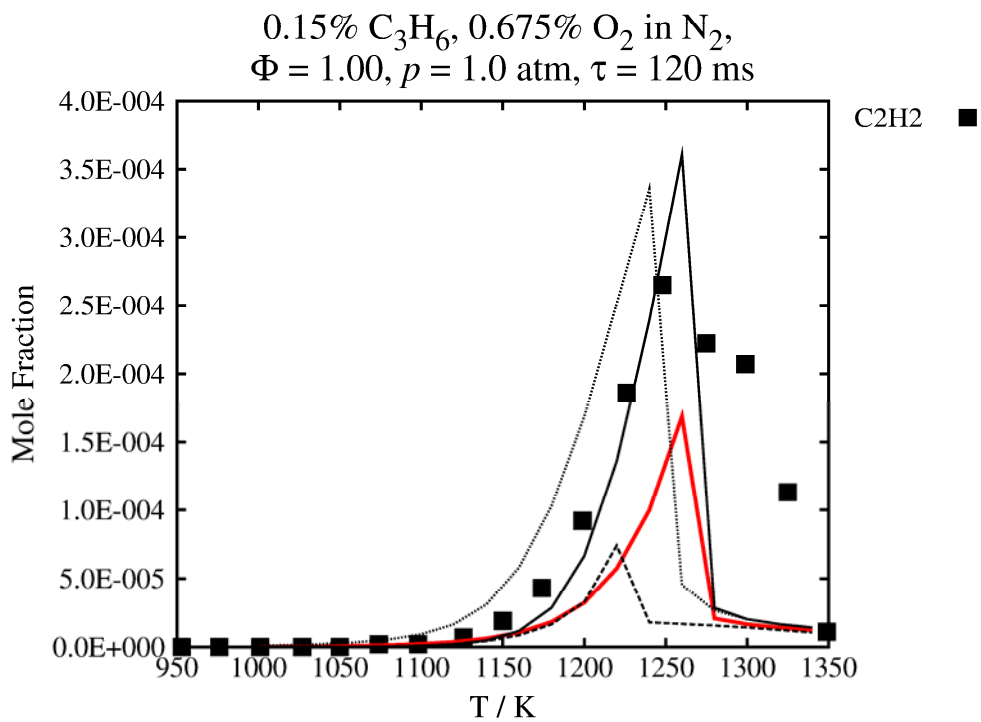
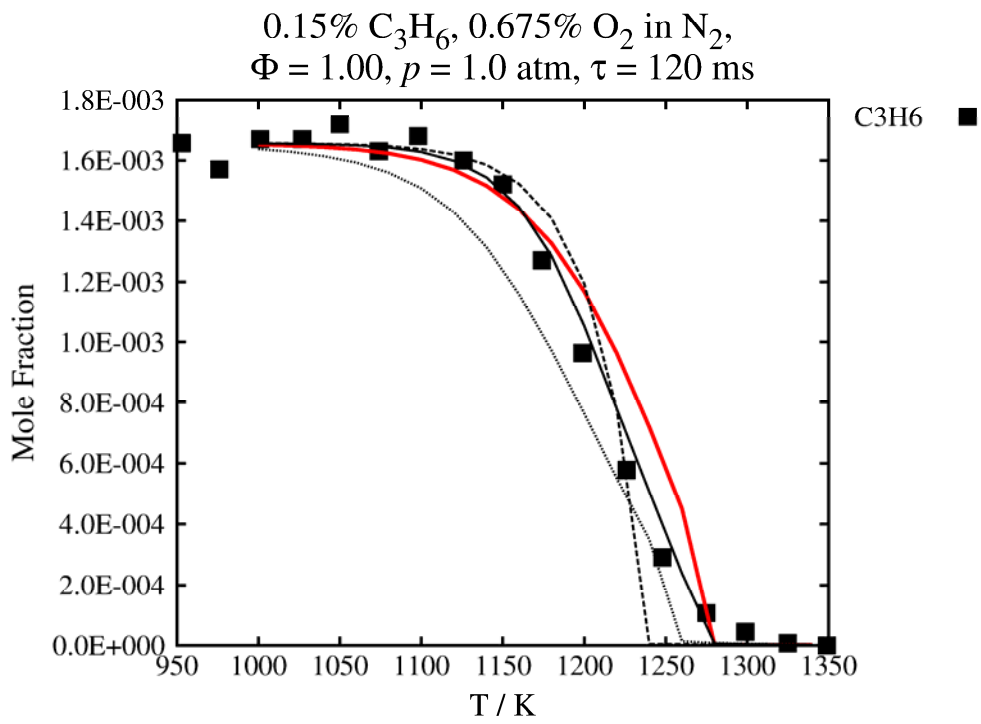
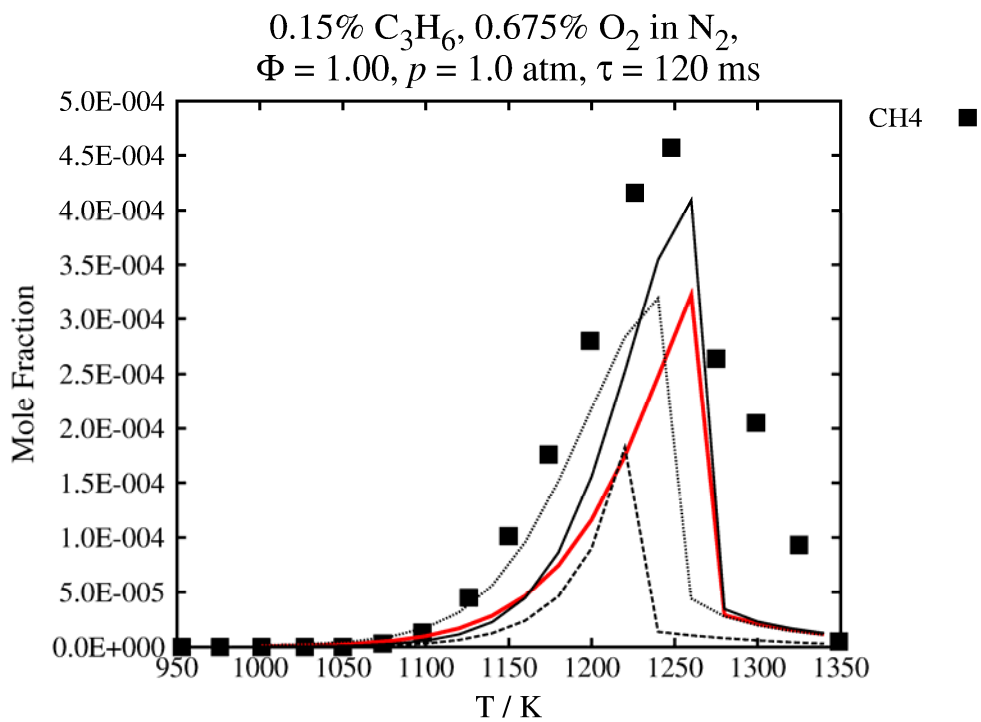
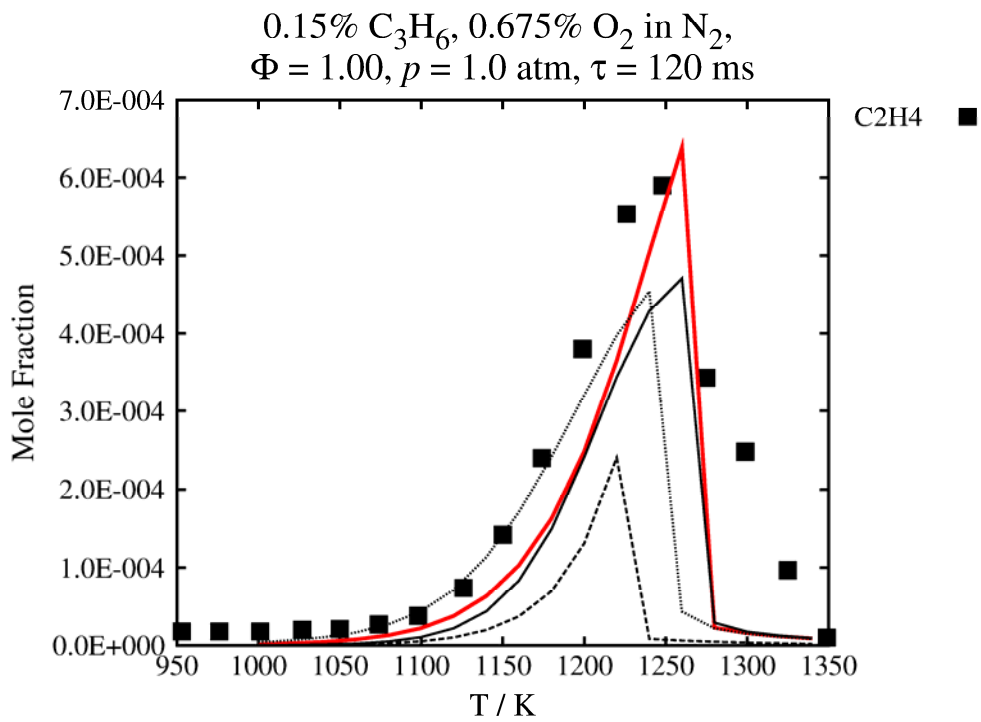
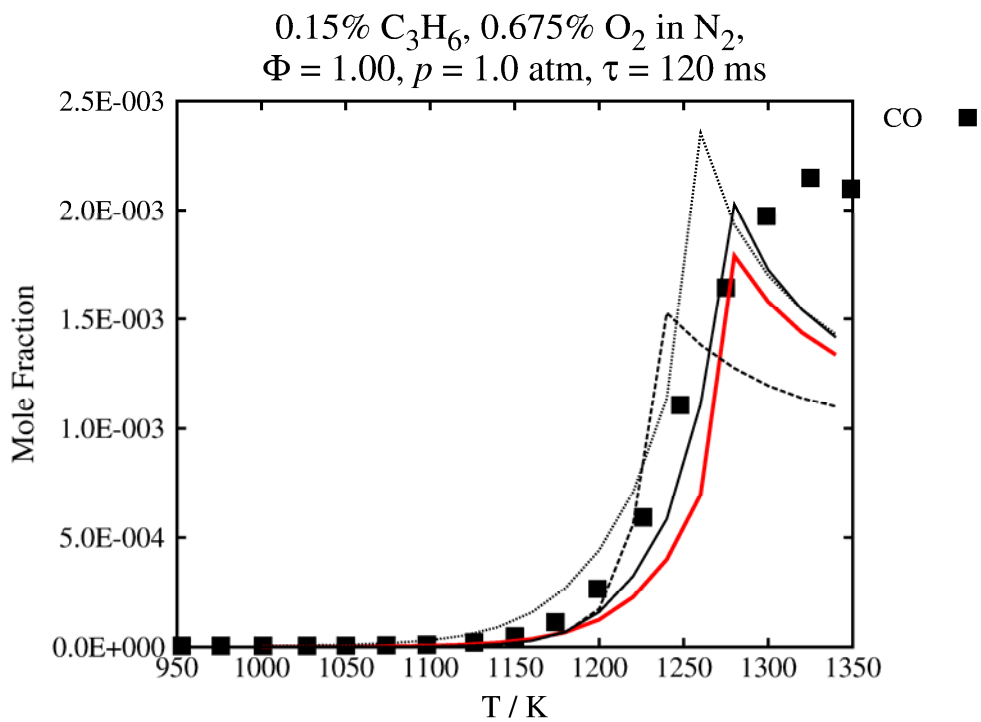
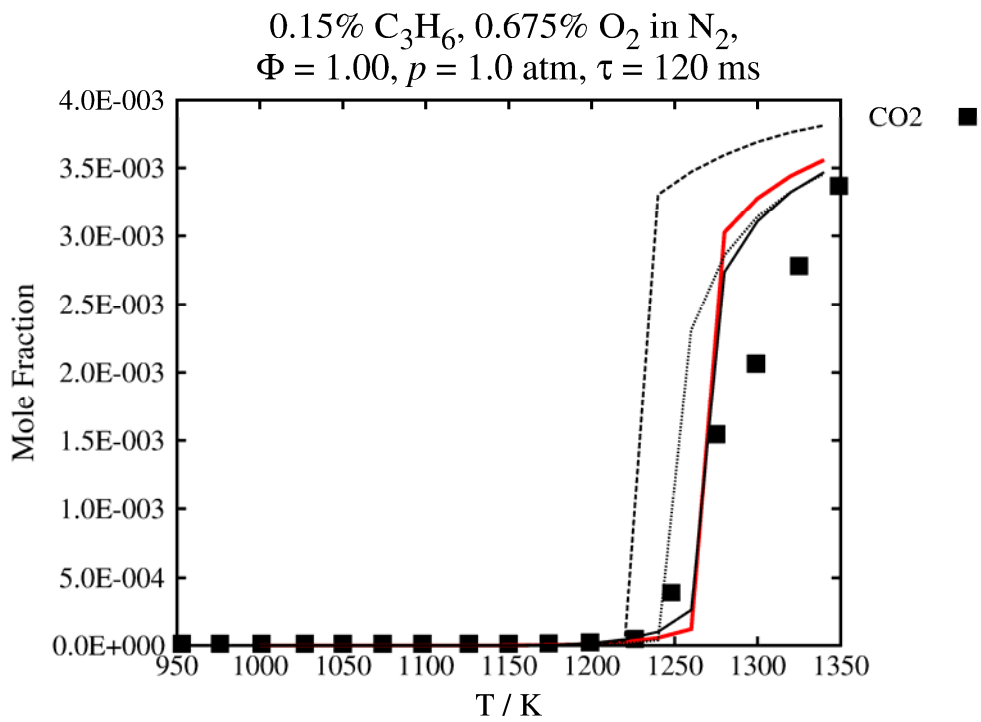


Figure 11 Jet-stirred reactor of propene/O₂/N₂. Symbols are experimental data [5] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].







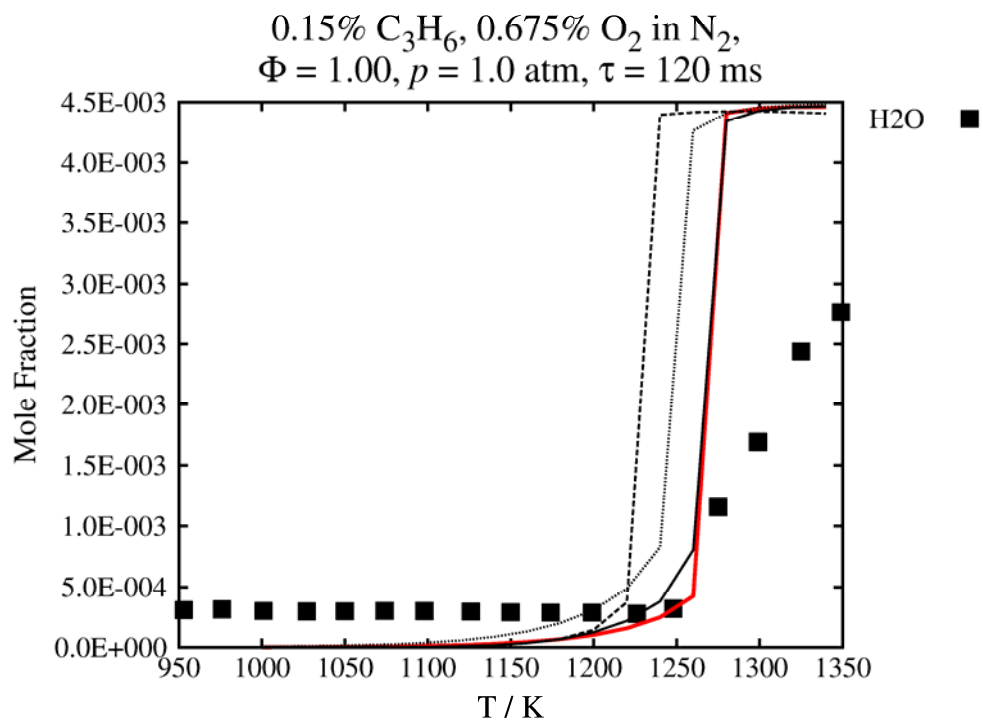
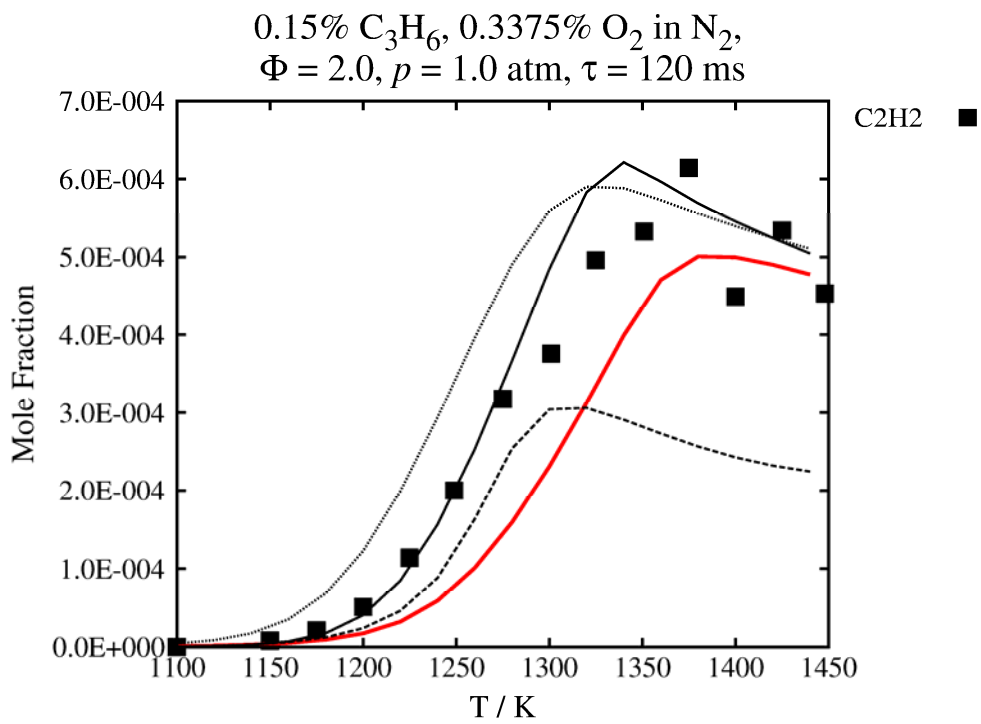
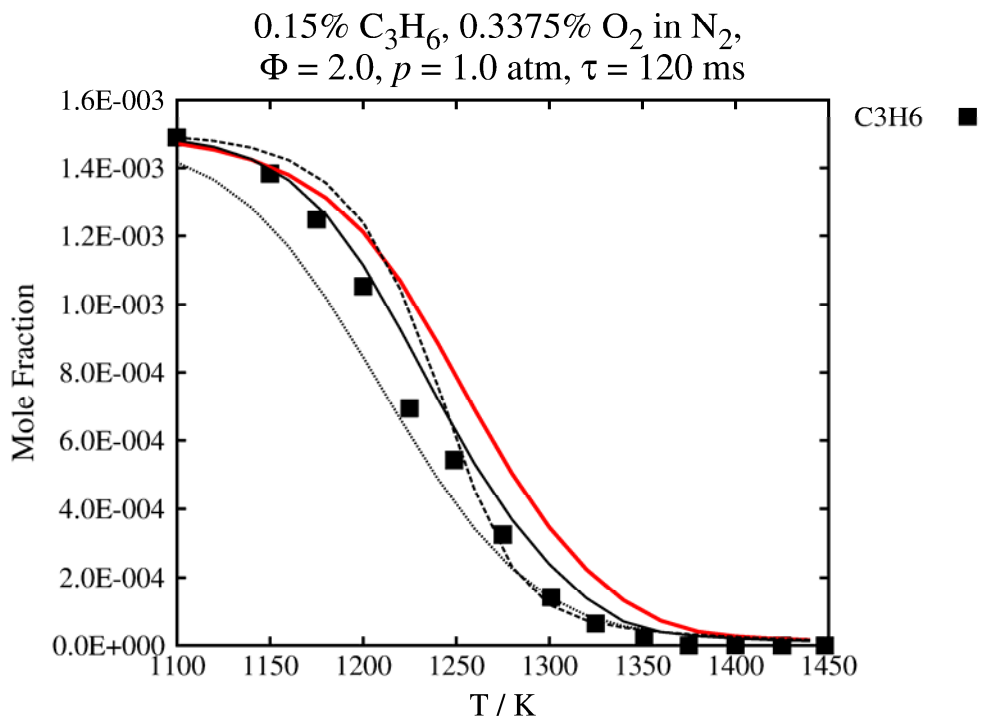
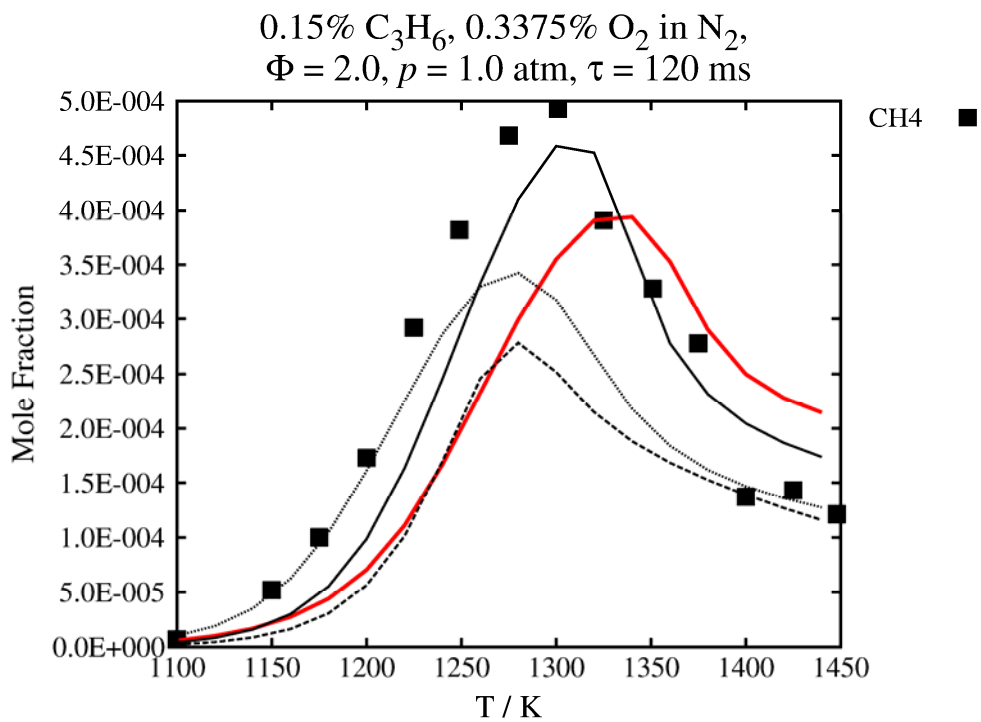
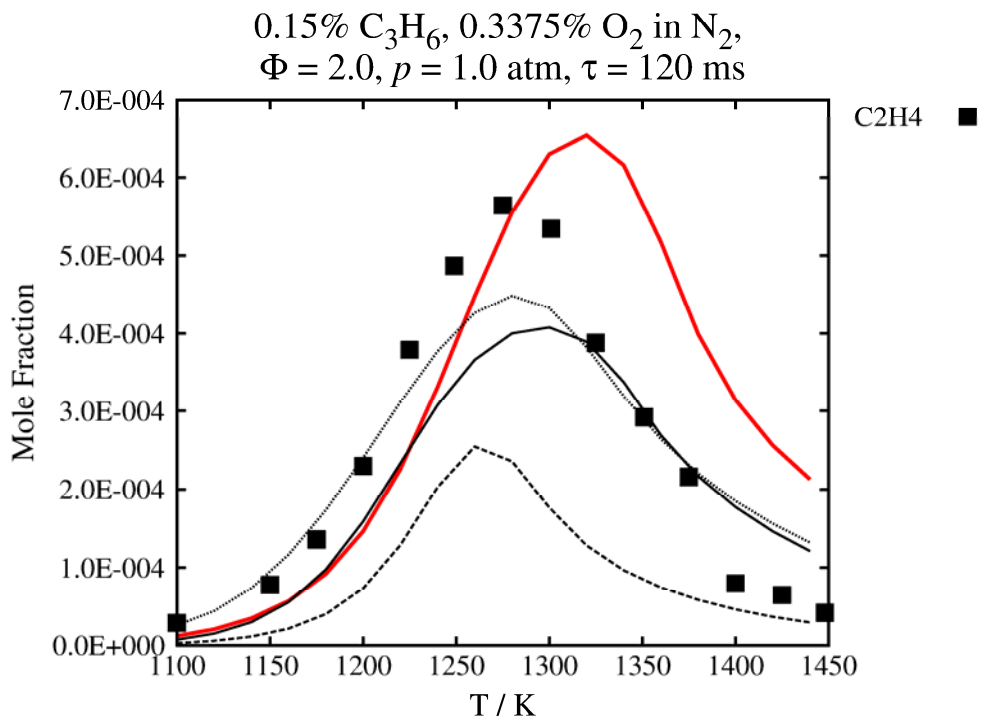
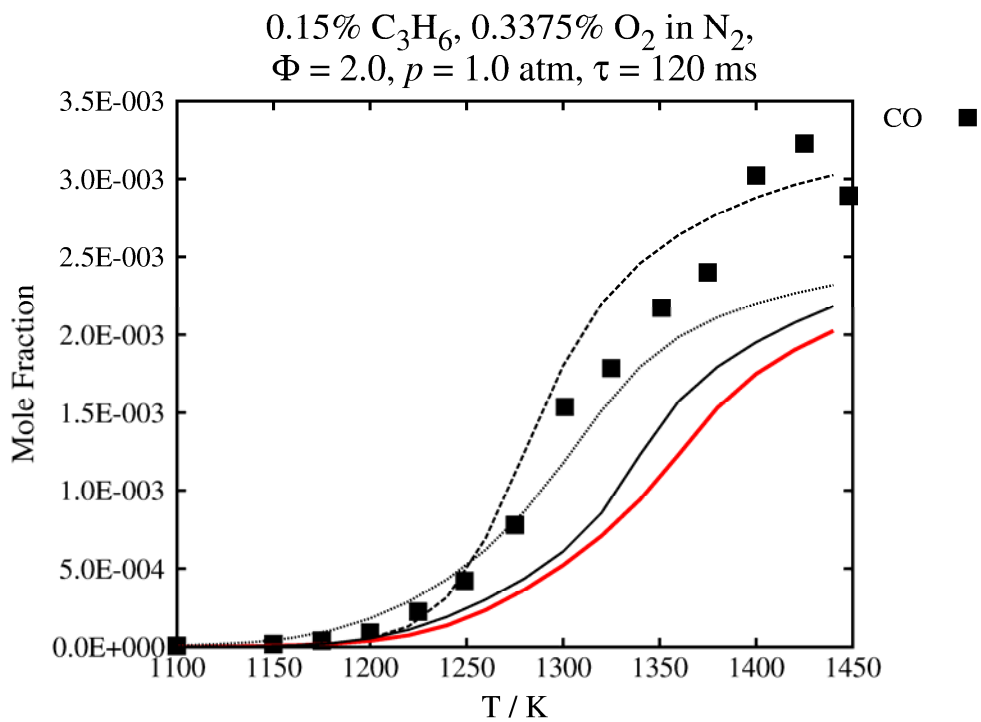
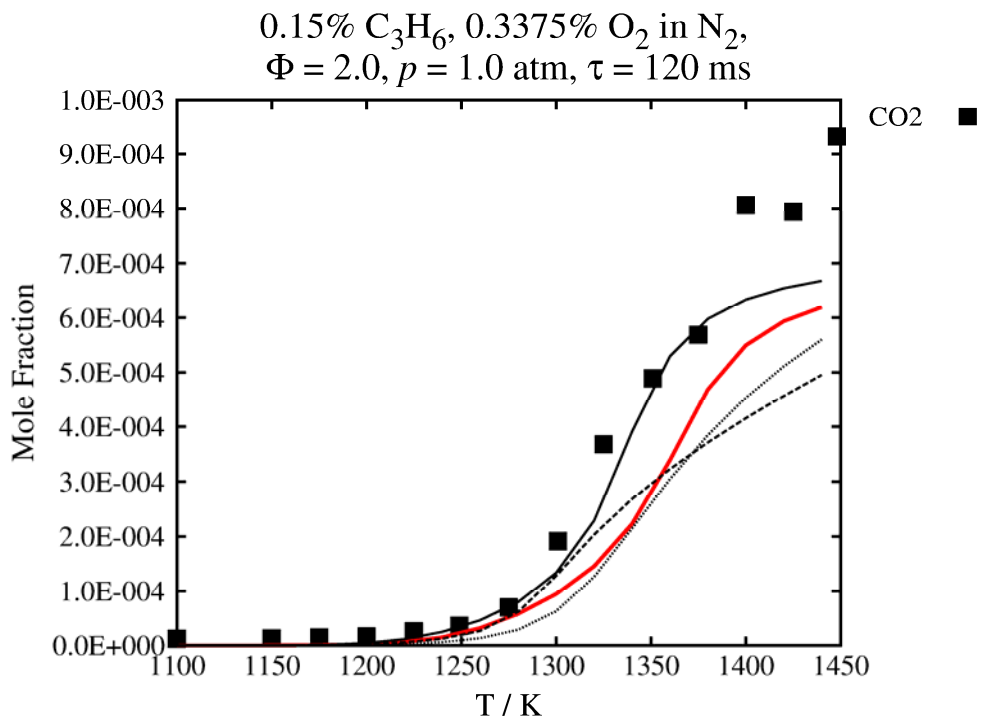


Figure 12 Jet-stirred reactor of propene/O₂/N₂. Symbols are experimental data [5] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].







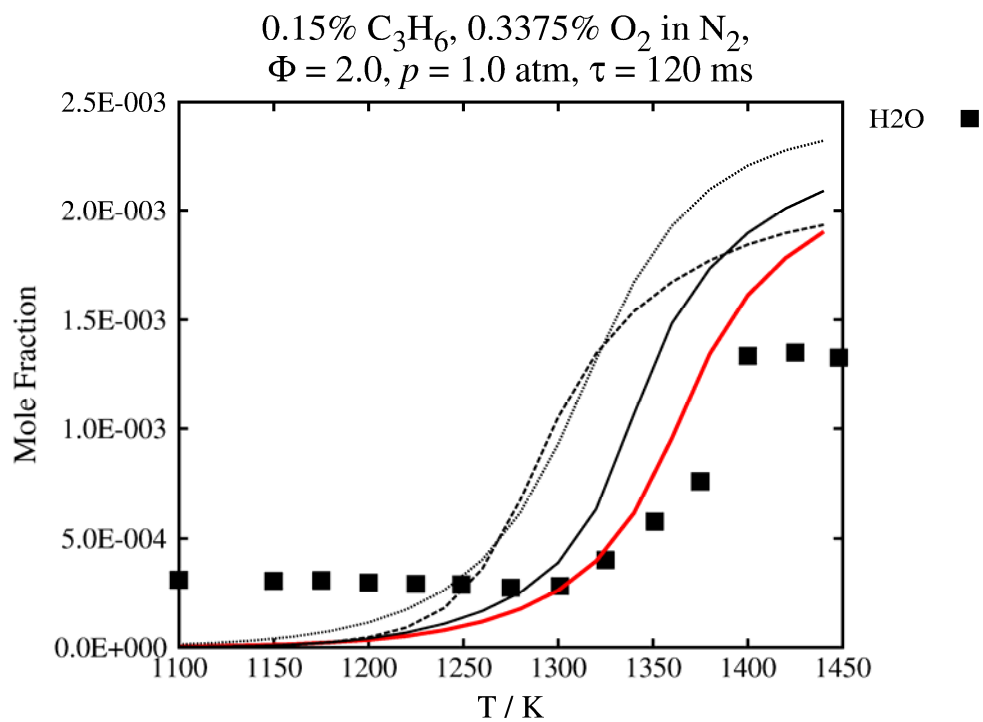
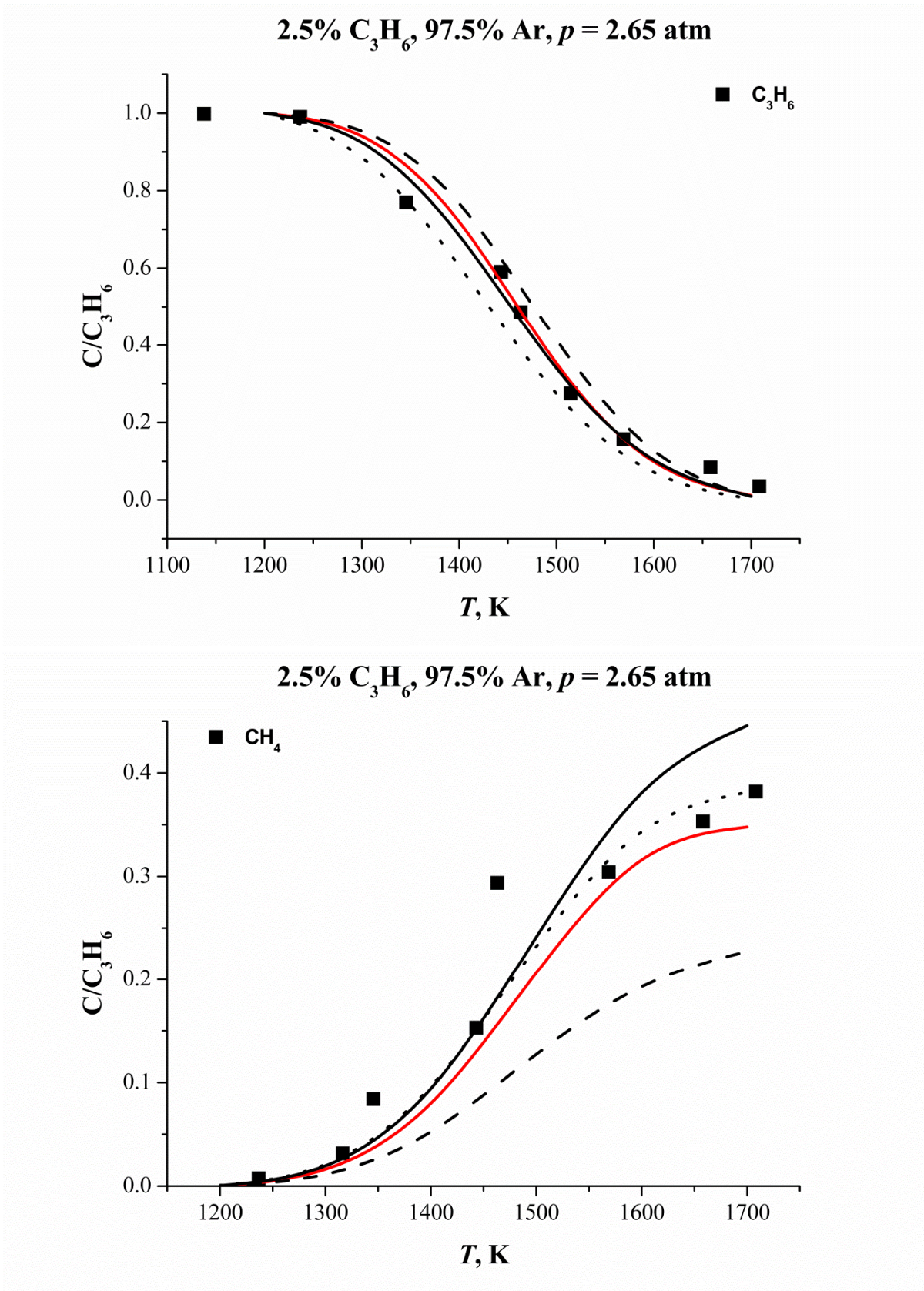
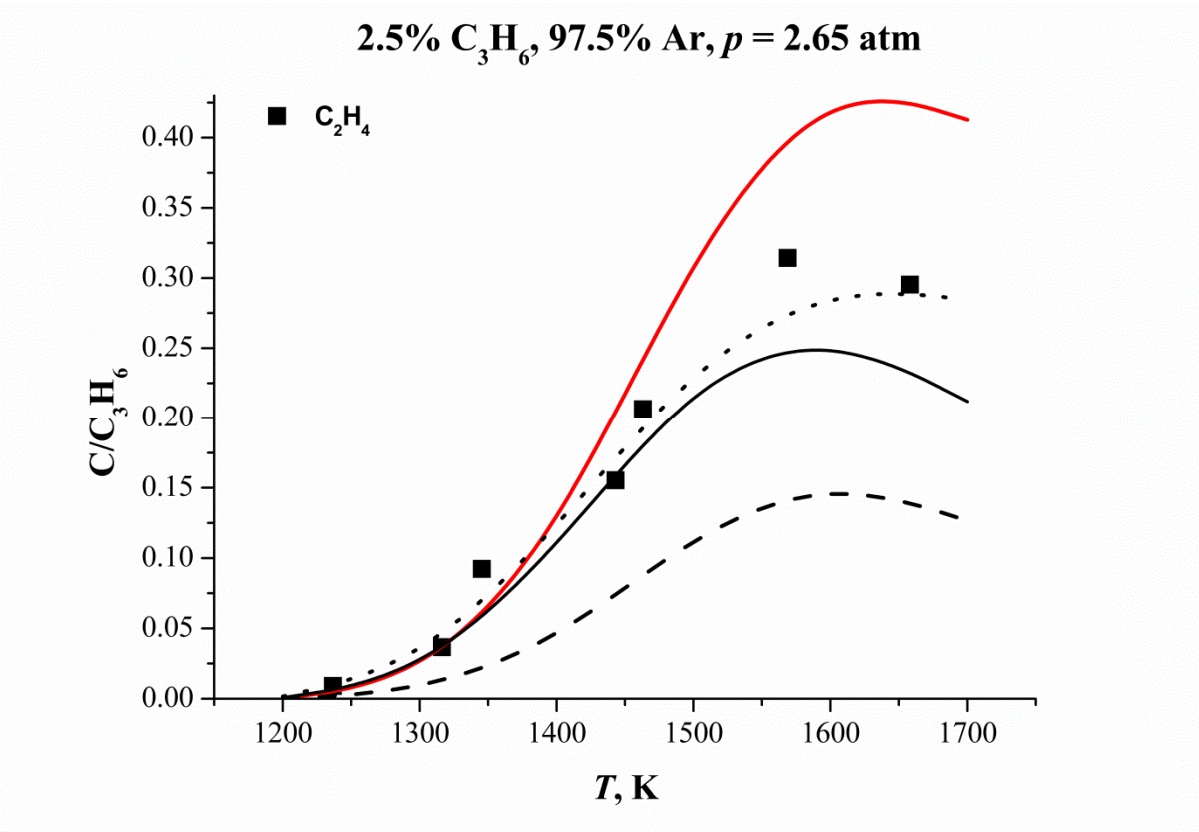
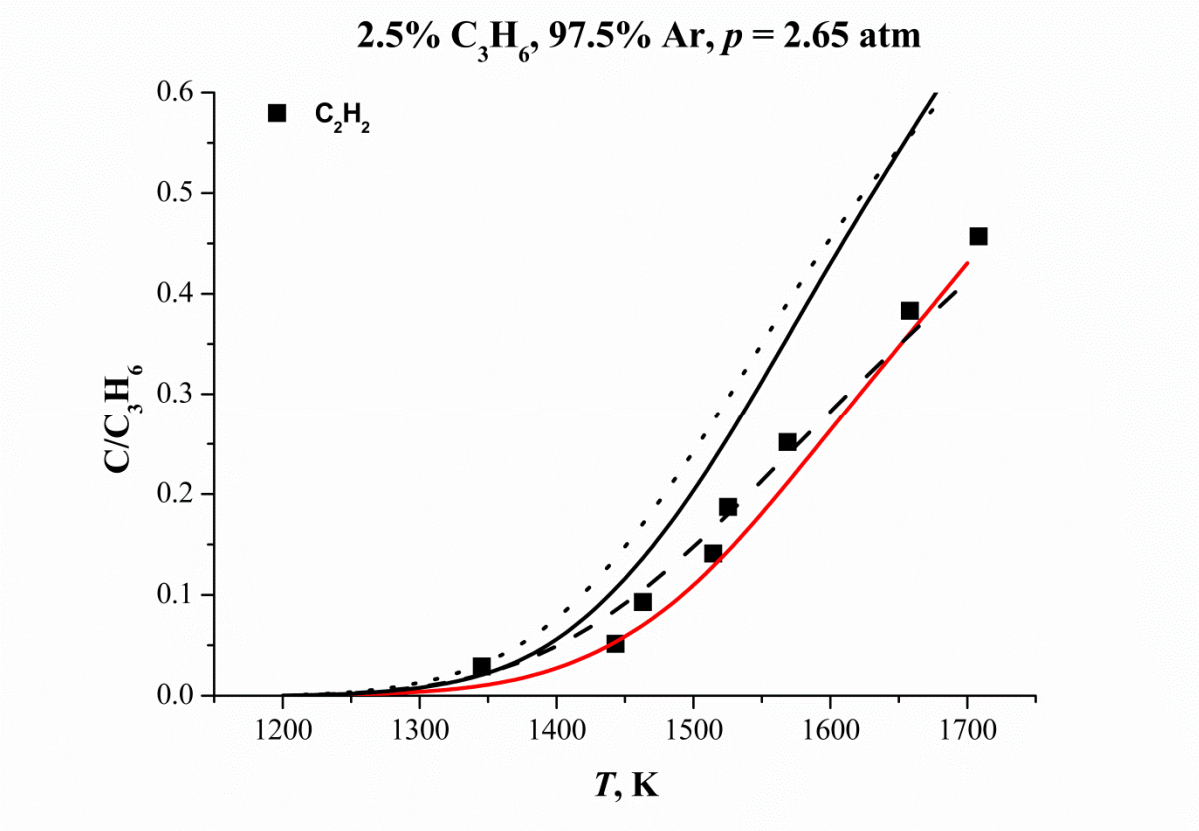


Figure 13 Jet-stirred reactor of propene/O₂/N₂. Symbols are experimental data [5] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

Shock tube

Hidaka et al.[6]





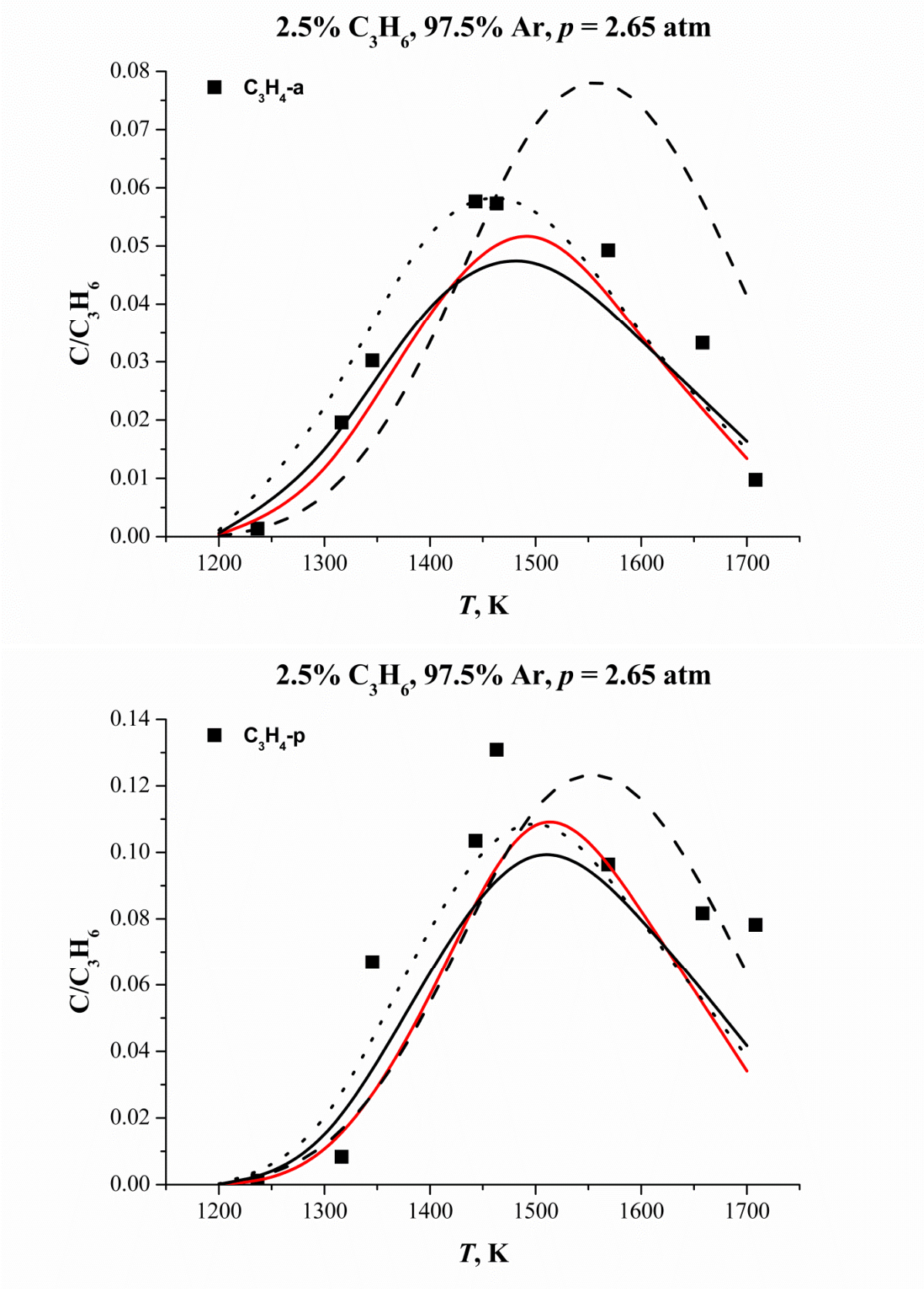
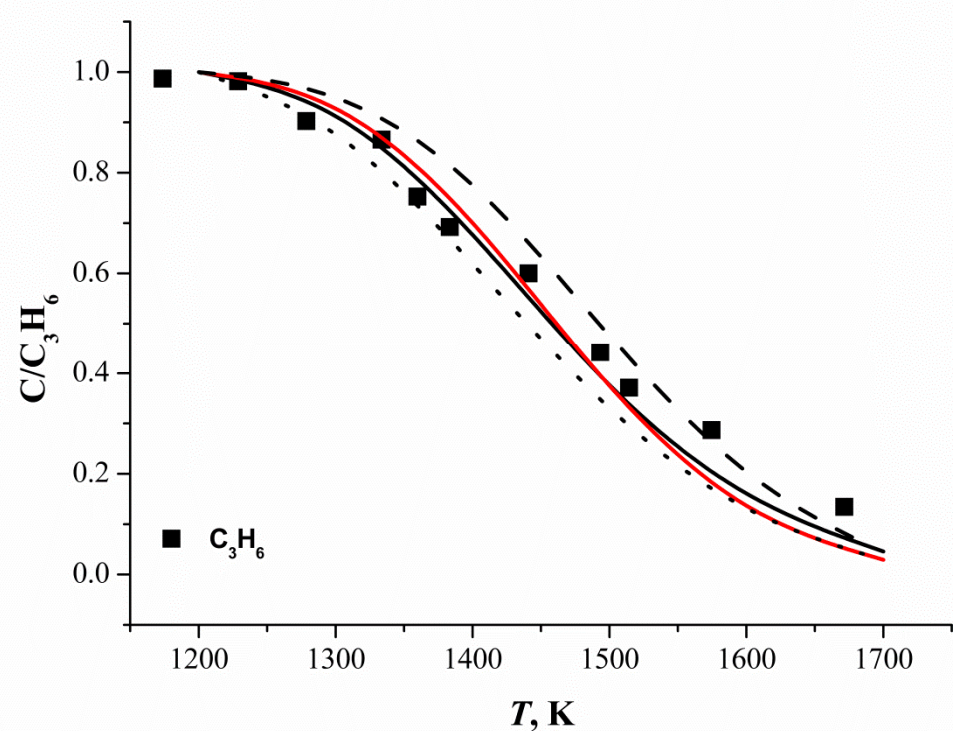
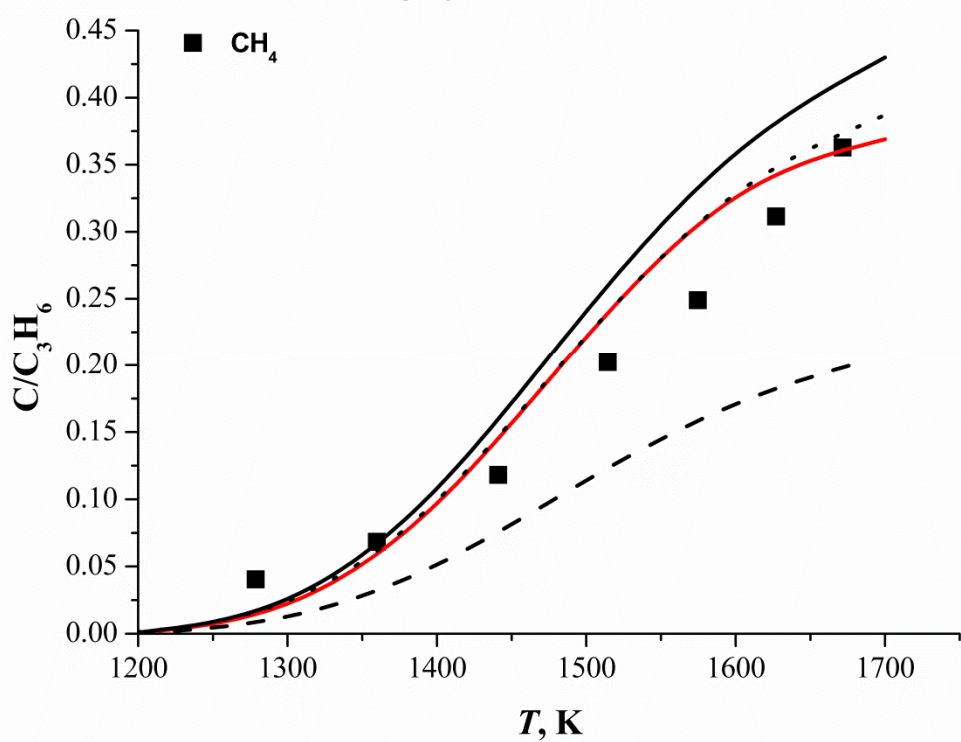


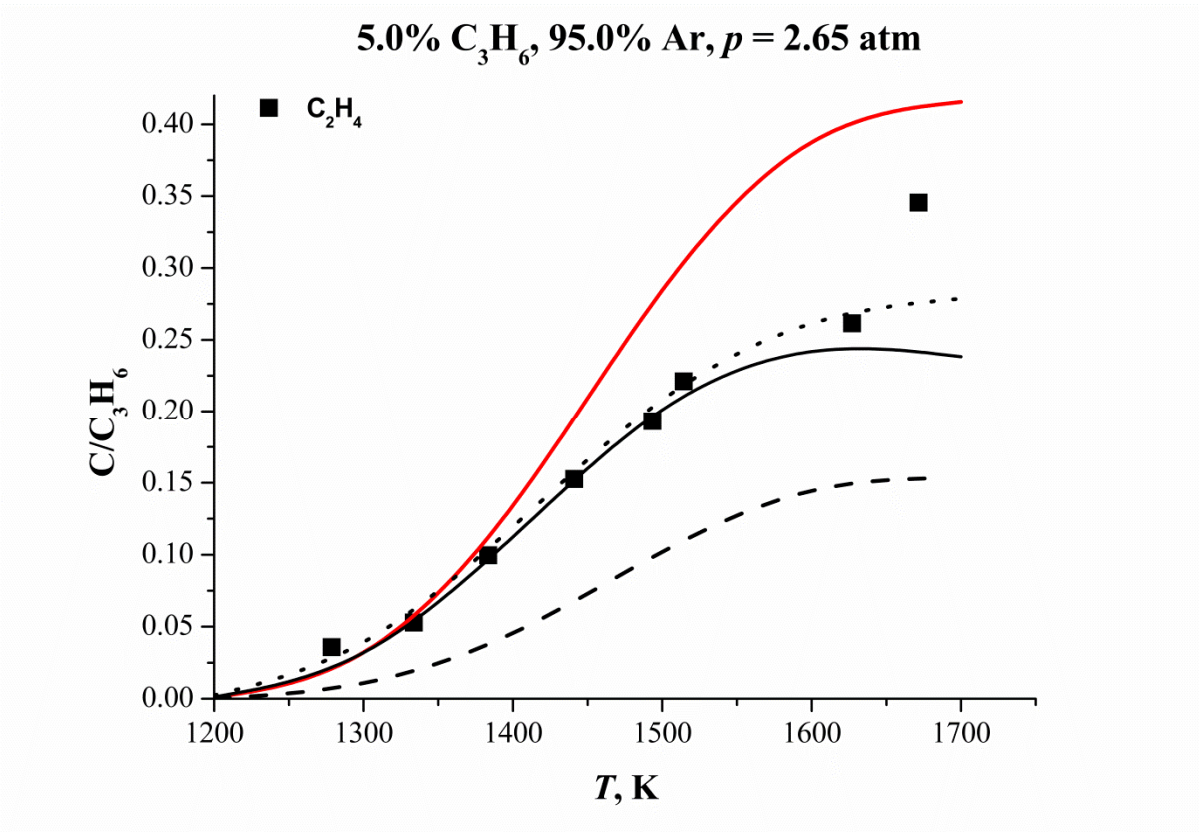
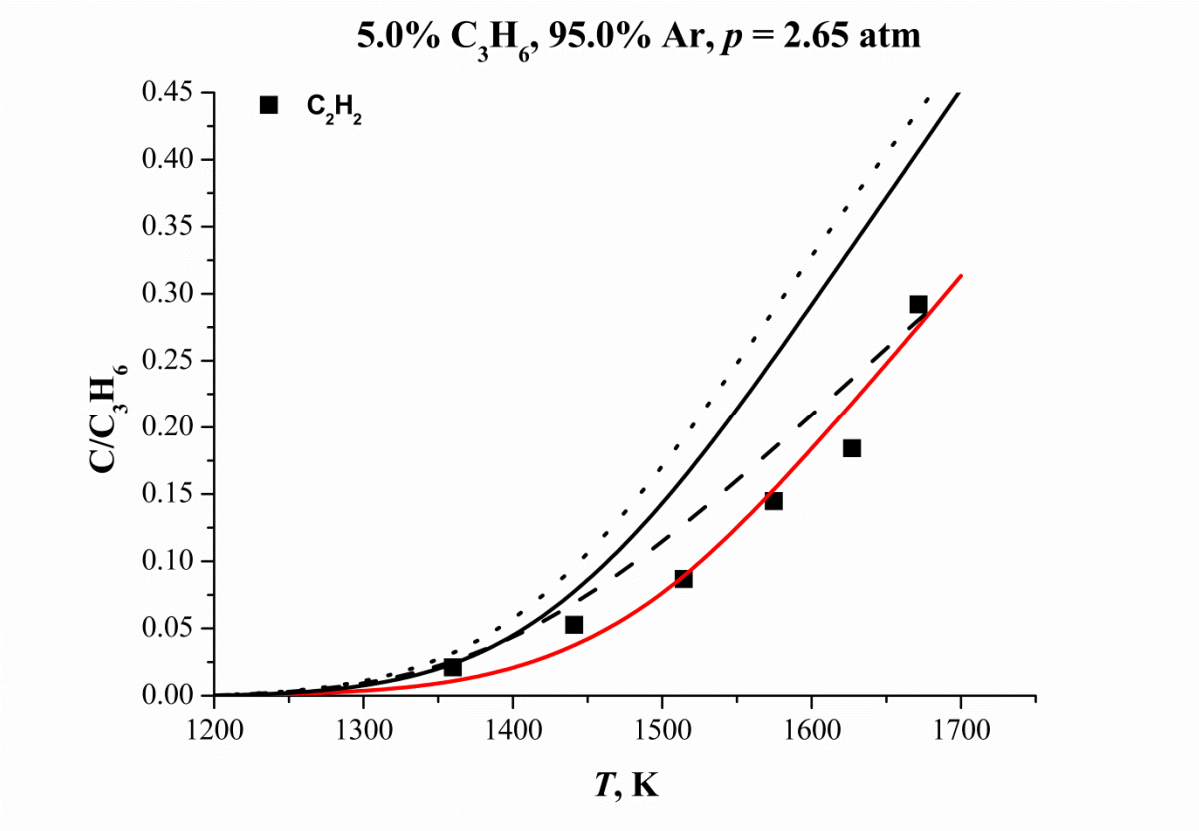
Figure 14 Shock tube, propene/Ar. Symbols are experimental data [6] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], •• • USC II[3].

5.0% C₃H₆, 95.0% Ar, $p = 2.65$ atm

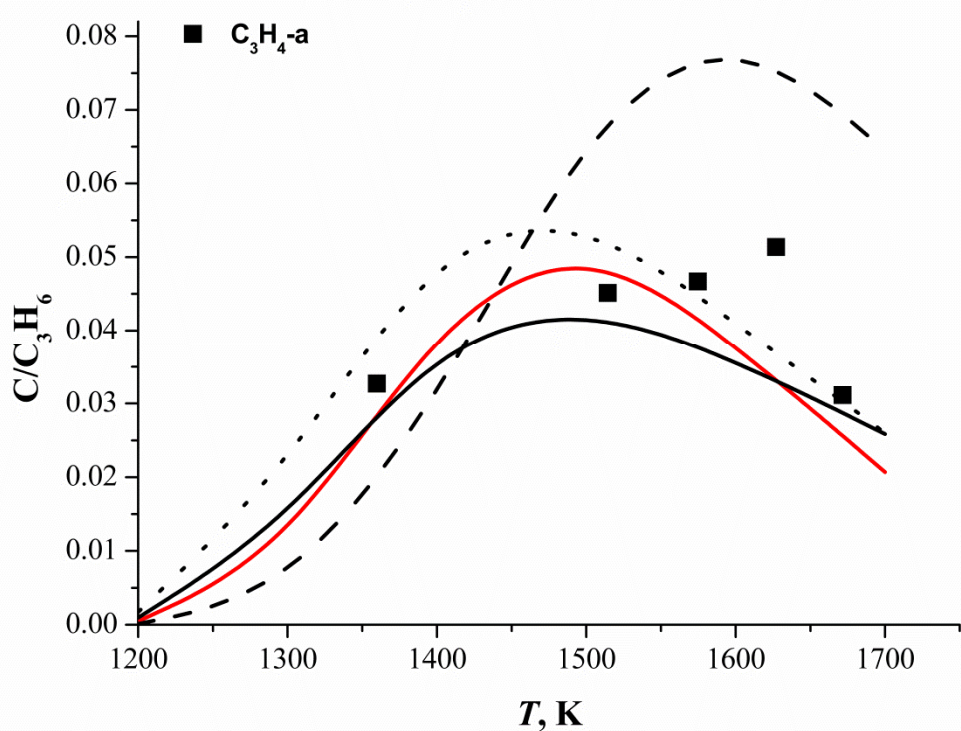


5.0% C₃H₆, 95.0% Ar, $p = 2.65$ atm

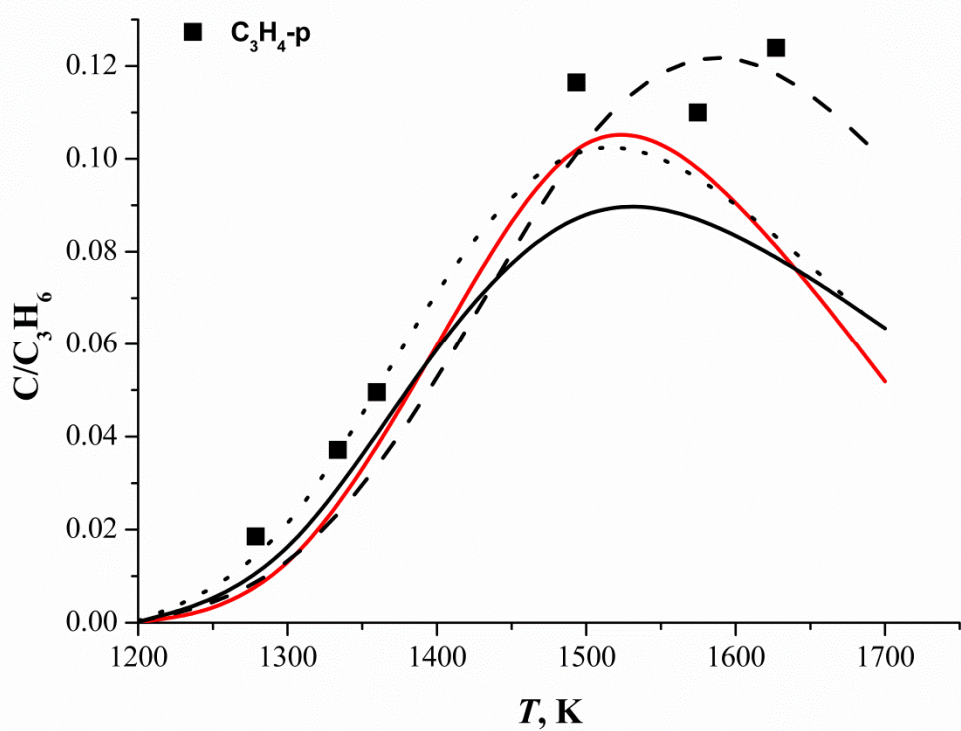




5.0% C₃H₆, 95.0% Ar, $p = 2.65$ atm



5.0% C₃H₆, 95.0% Ar, $p = 2.65$ atm



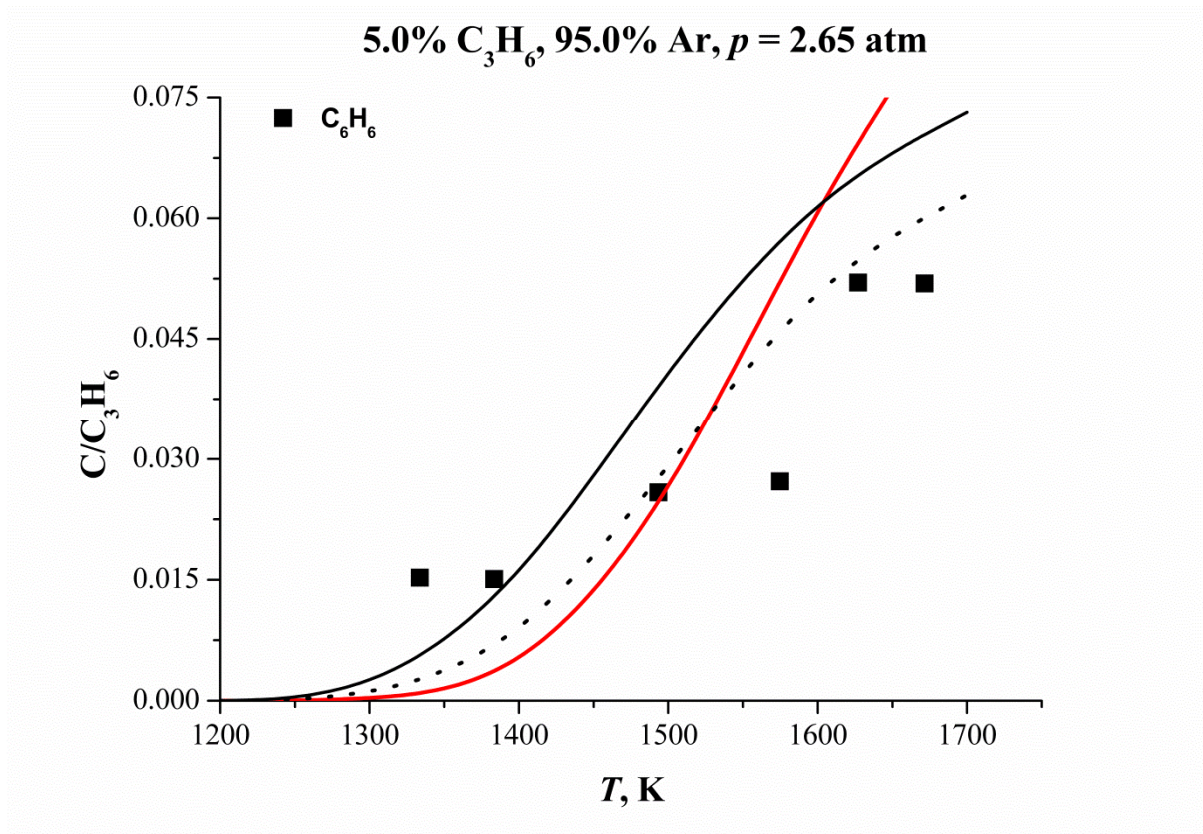
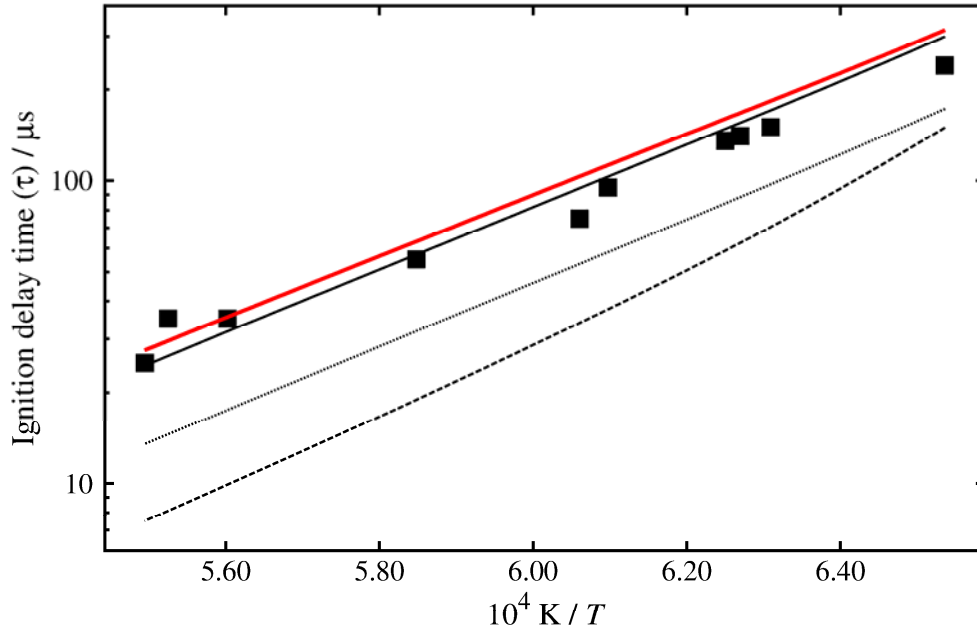
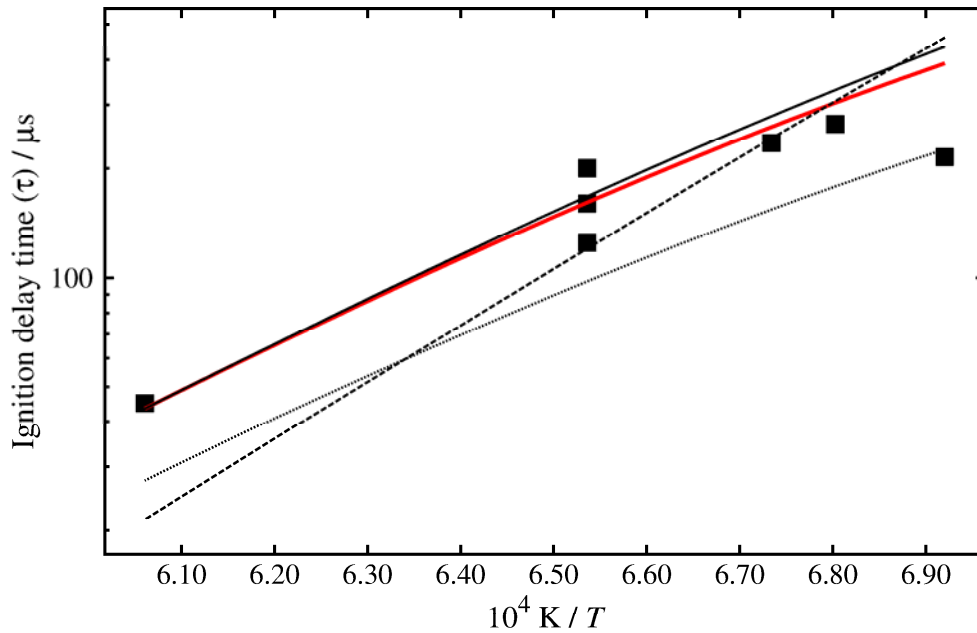


Figure 15 Shock tube, propene/Ar. Symbols are experimental data [6] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], • • • USC II[3].

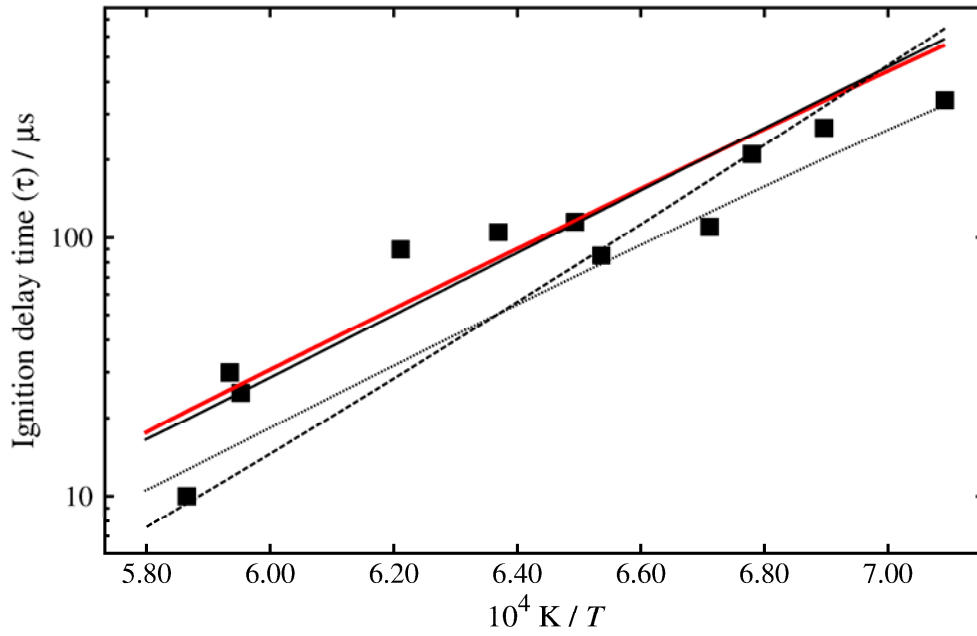
1.6% C₃H₆, 7.2% O₂, 91.2% Ar, $\Phi = 1.0$, $p_{av} = 1.9$ atm



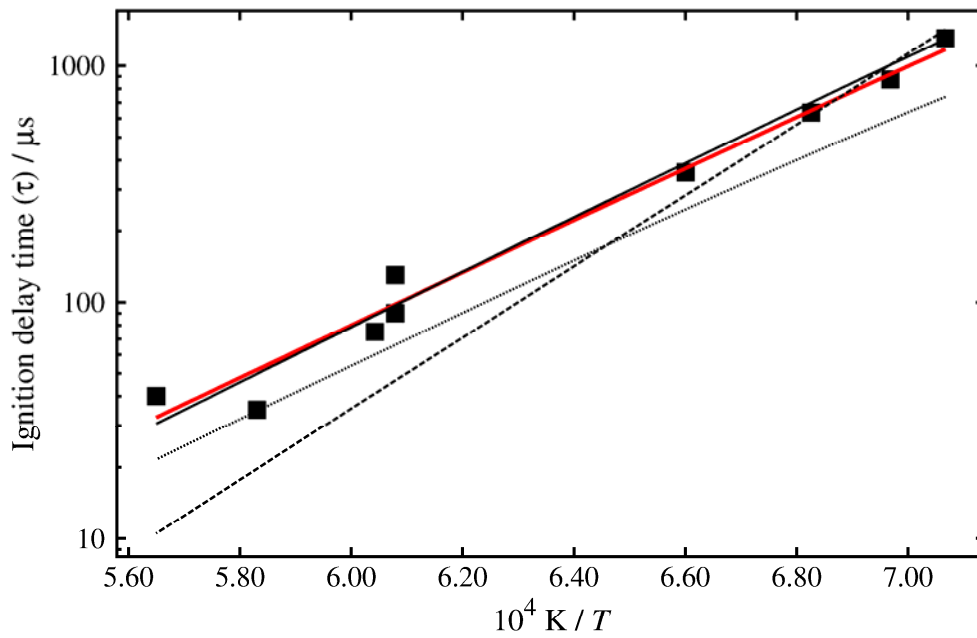
1.6% C₃H₆, 7.2% O₂, 91.2% Ar, $\Phi = 1.0$, $p_{av} = 4.2$ atm



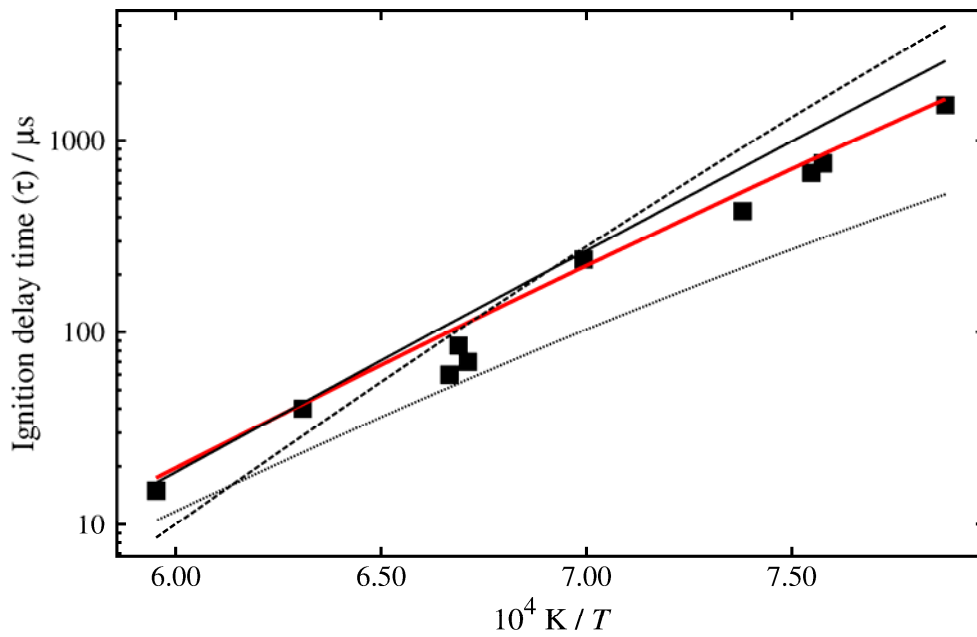
0.8% C₃H₆, 7.2% O₂, 92.0% Ar, $\Phi = 0.5$, $p_{av} = 3.8$ atm



1.6% C₃H₆, 3.6% O₂, 94.8% Ar, $\Phi = 2.0$, $p_{av} = 4.1$ atm



1.6% C₃H₆, 14.4% O₂, 84.0% Ar, $\Phi = 0.5$, $p_{av} = 3.9$ atm



3.2% C₃H₆, 7.8% O₂, 89.0% Ar, $\Phi = 1.8$, $p_{av} = 3.9$ atm

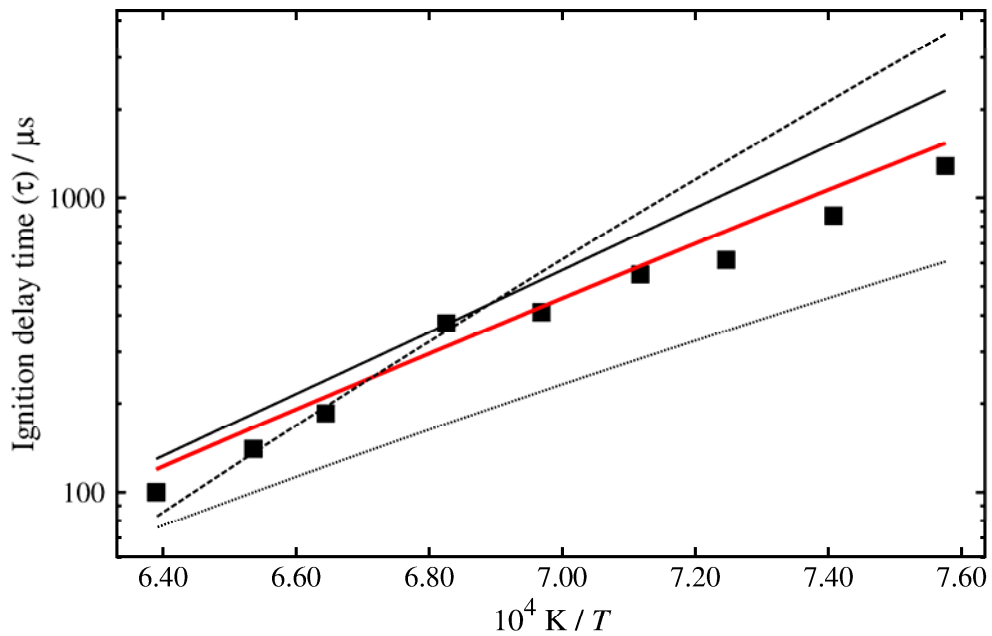


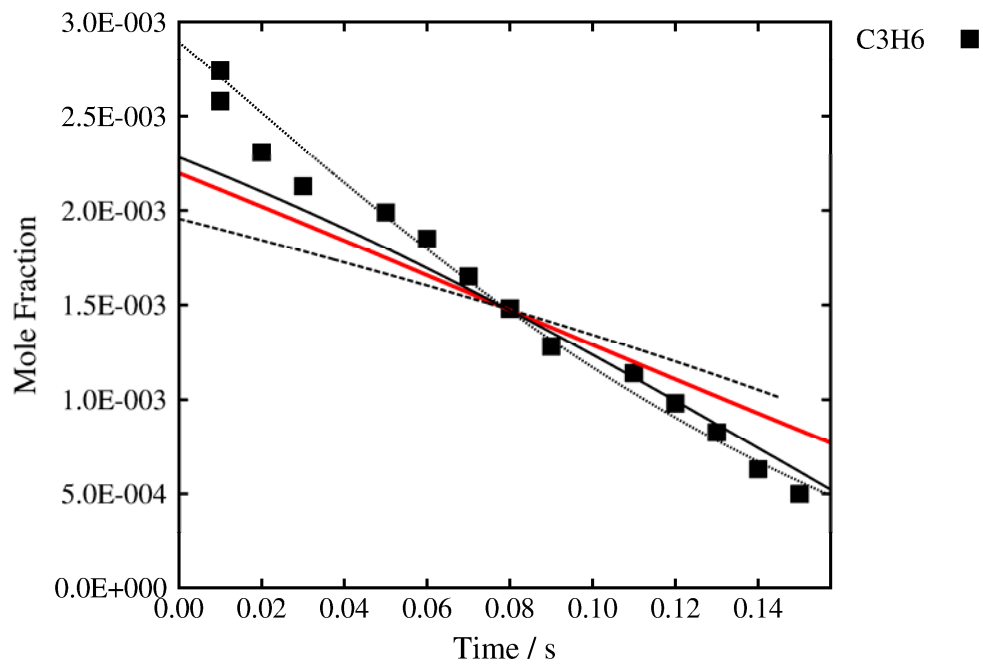
Figure 16 Shock tube ignition delay times of propene/O₂/Ar. Symbols are experimental data [7] lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - -

- Heyberger et al. [2], ••• USC II[3].

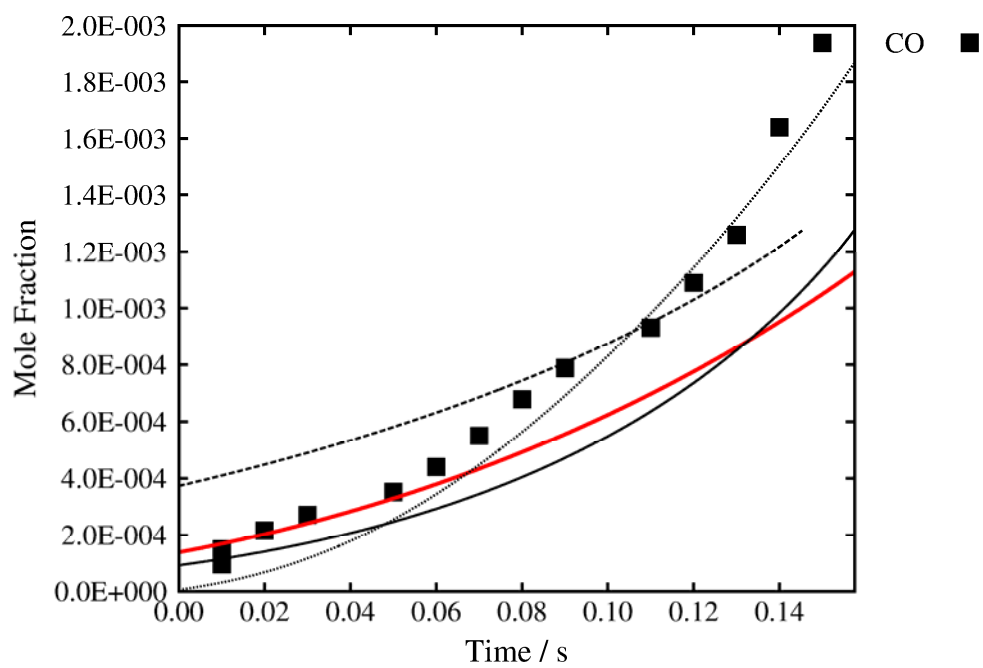
Flow reactor

Davis et al.[3]

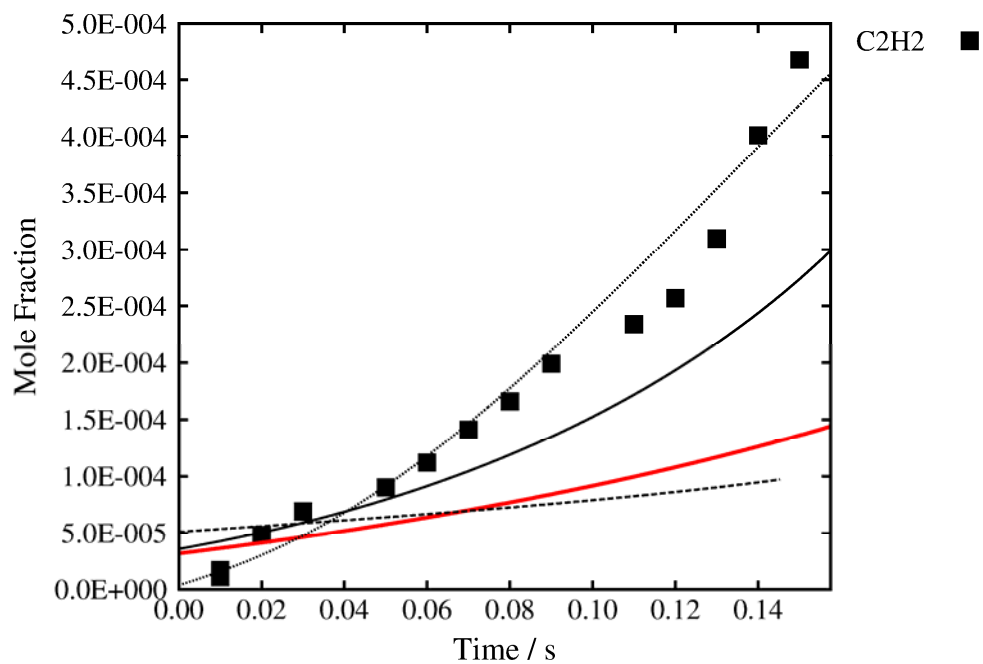
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



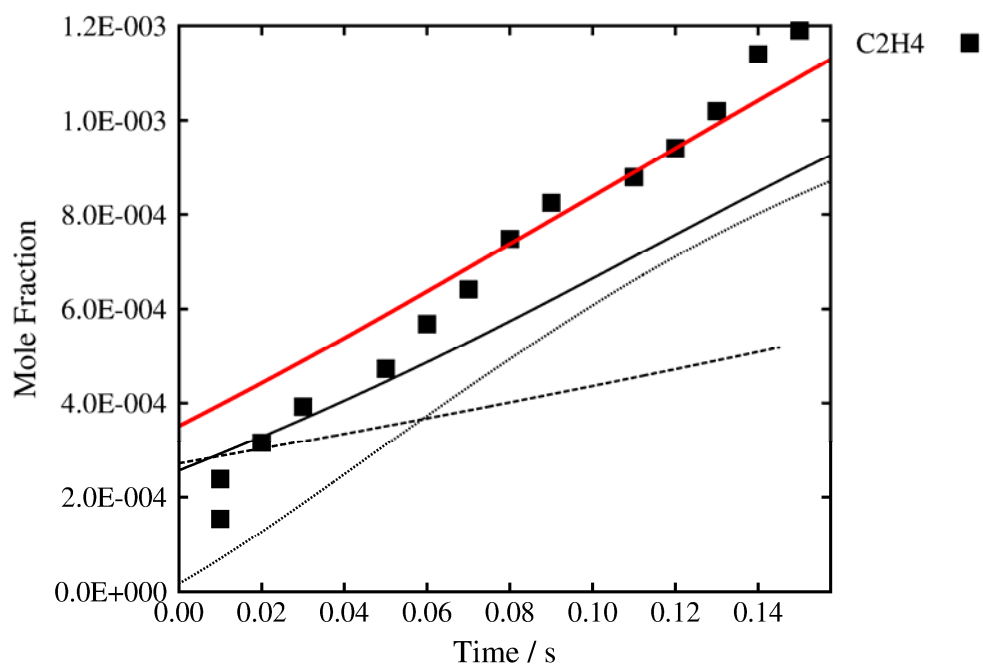
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



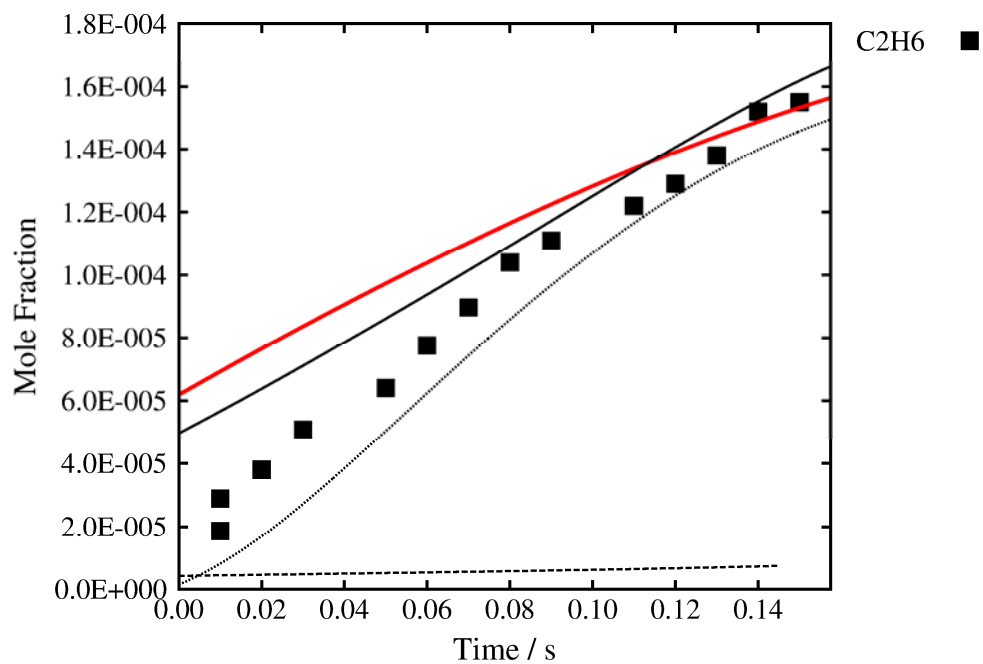
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



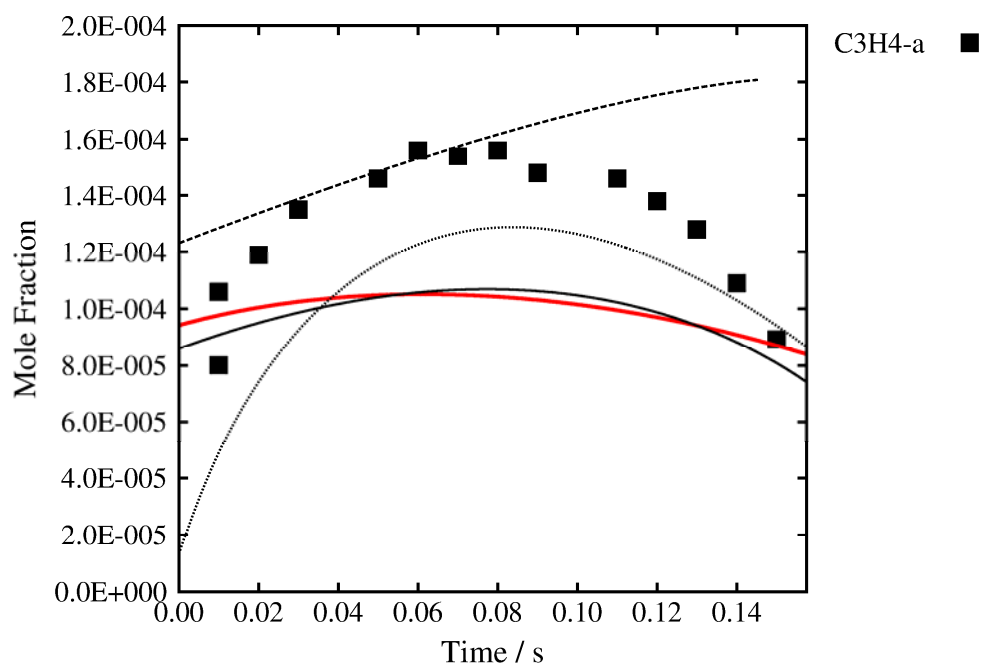
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



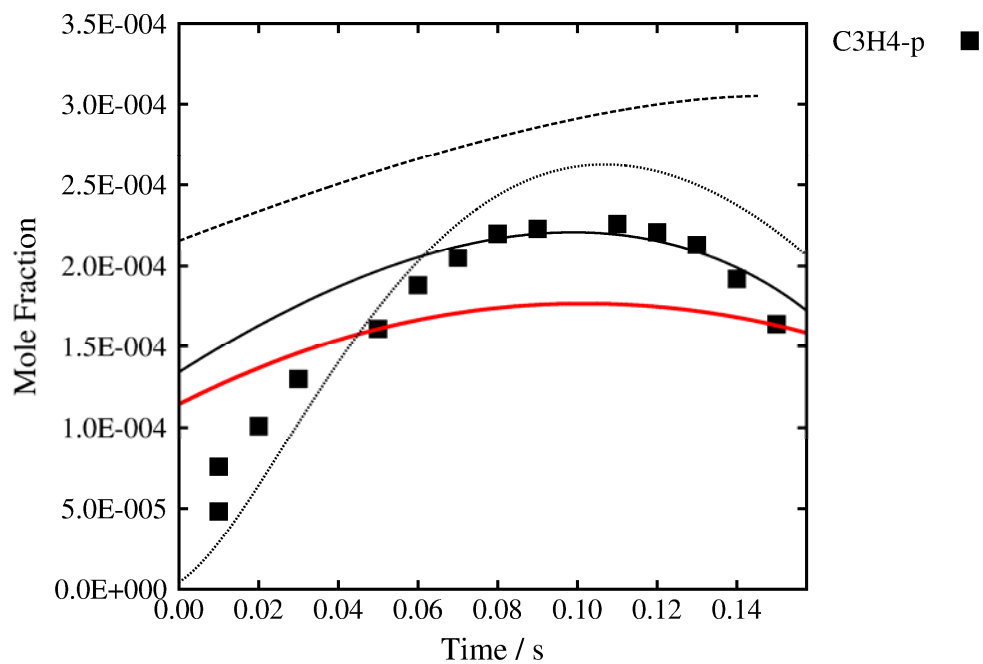
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



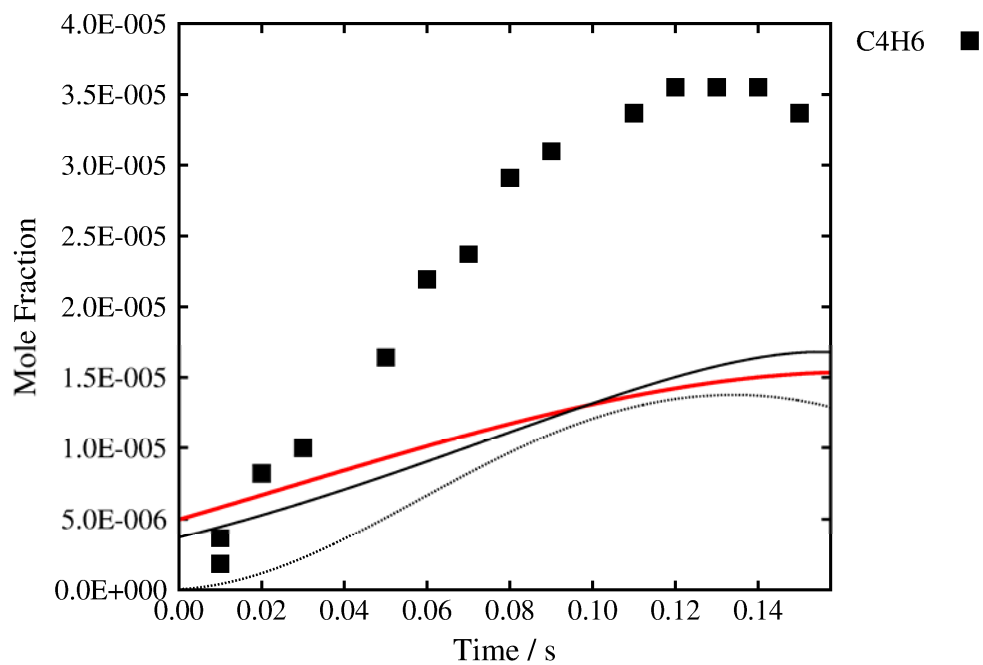
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



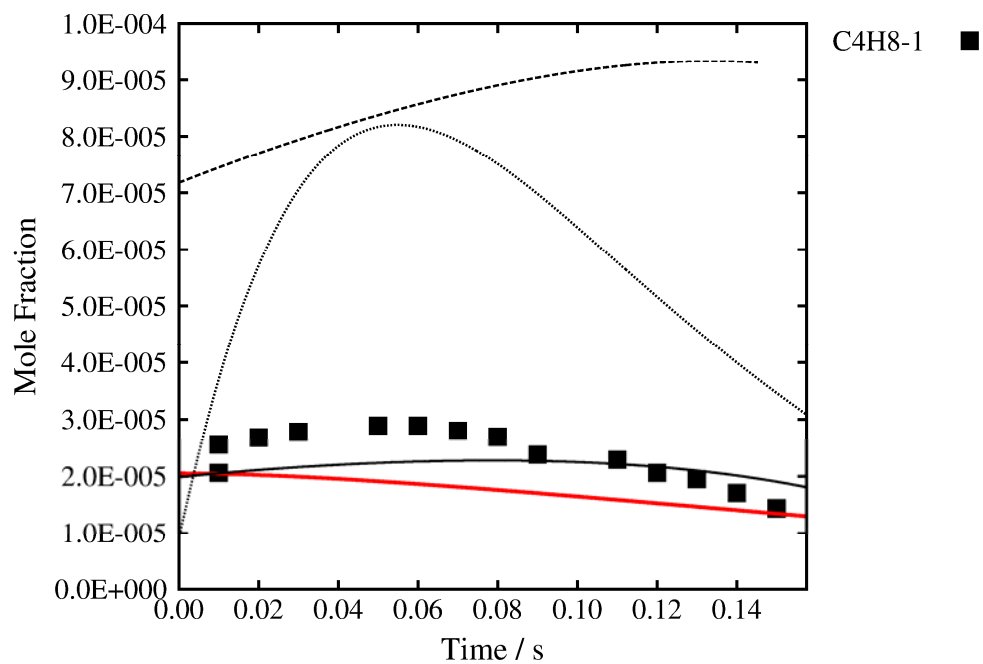
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



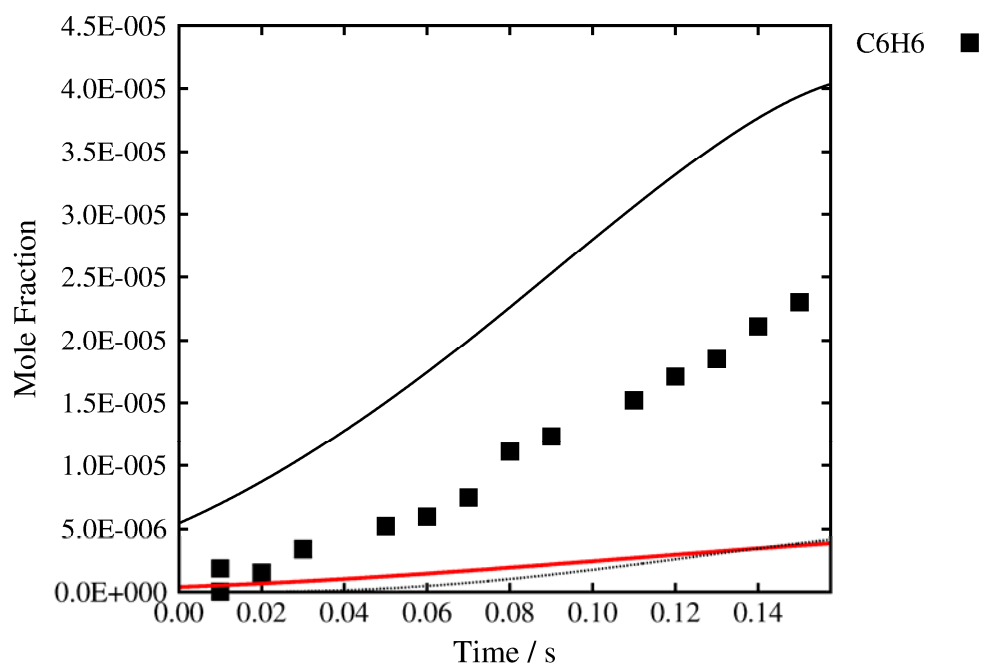
0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K



0.30% C₃H₆ 1.33% O₂ in N₂, $\Phi = 1.00$, $p = 1.0$ atm, $T = 1181$ K

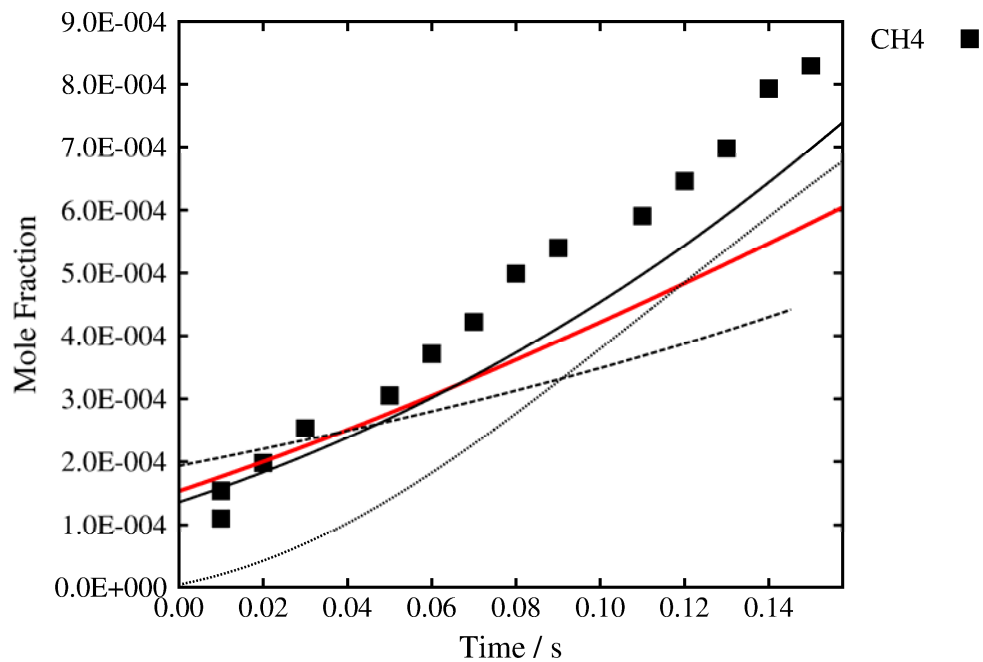
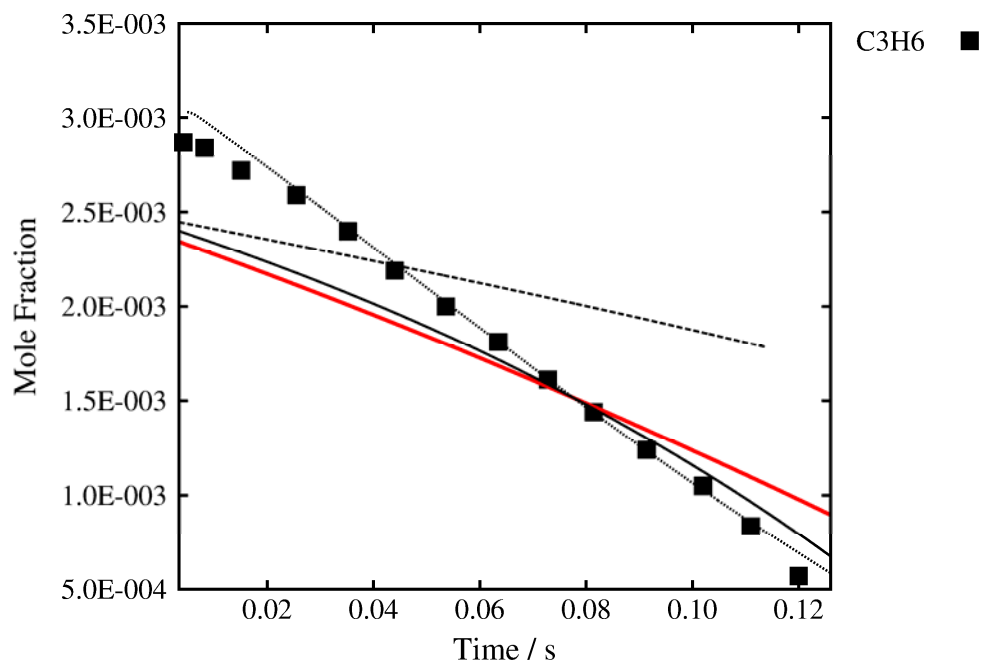
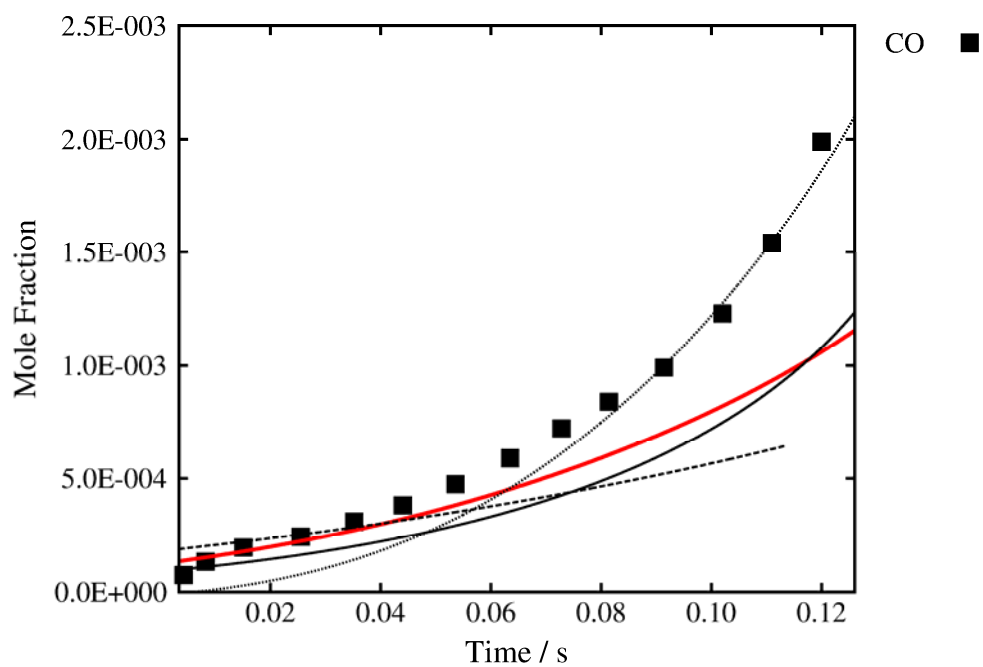


Figure 17 Flow reactor of propene/O₂/N₂. Symbols are experimental data [3] lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

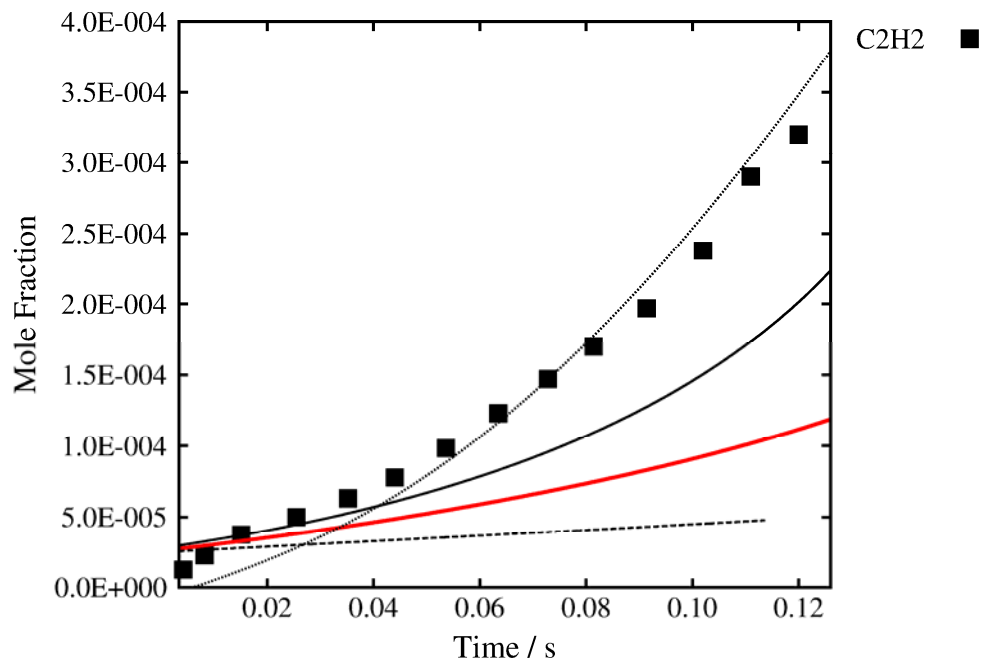
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



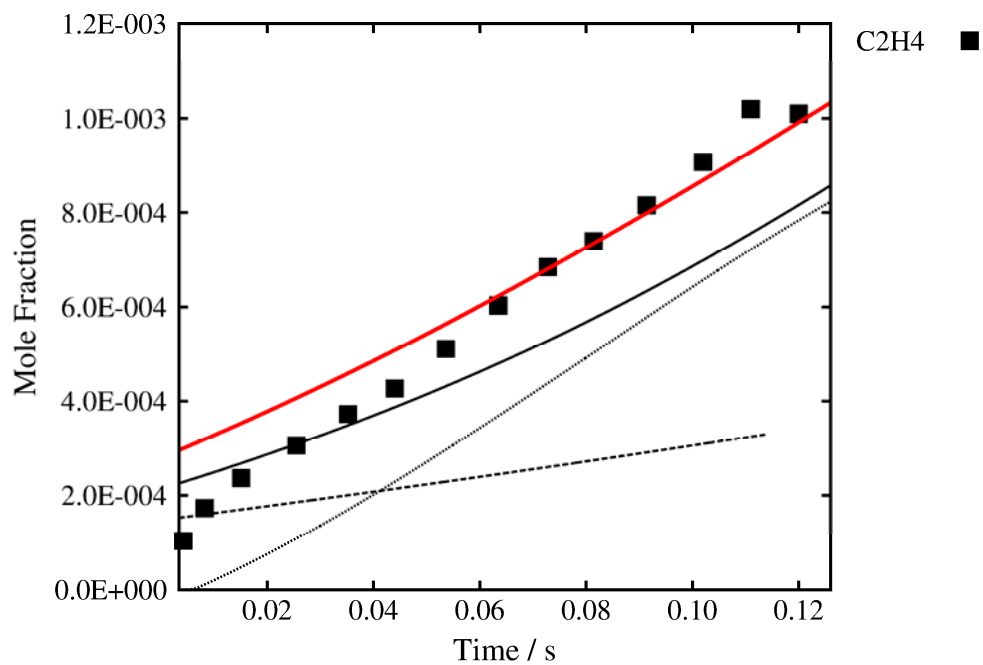
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



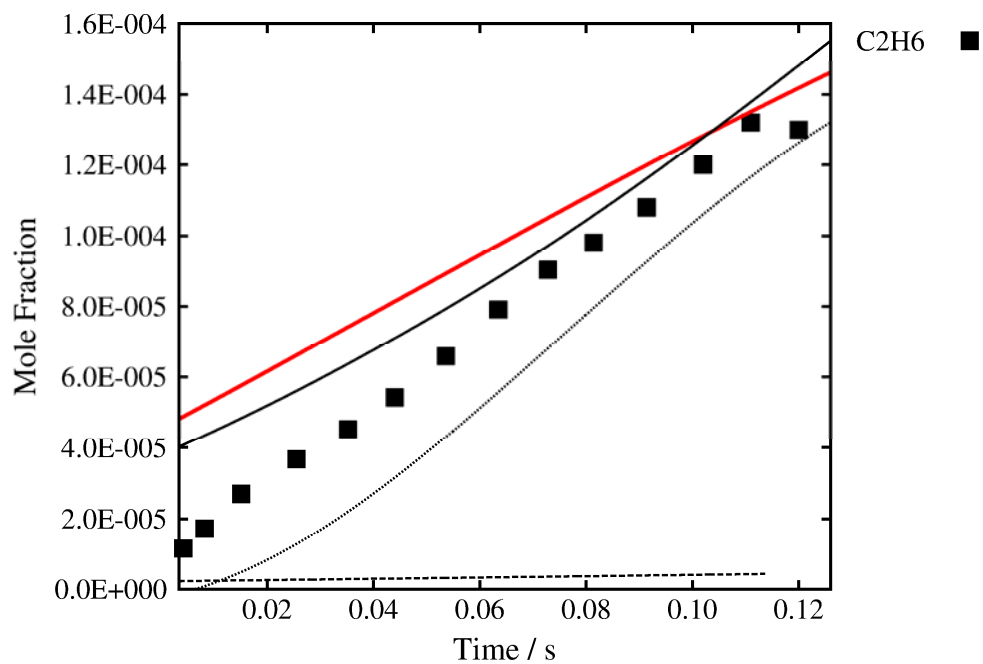
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



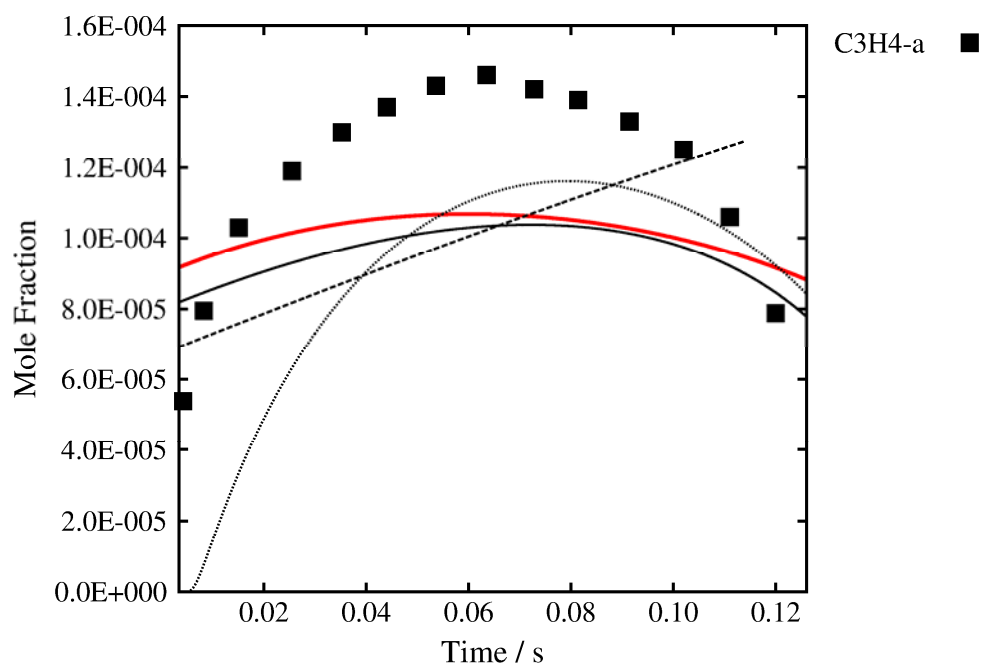
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



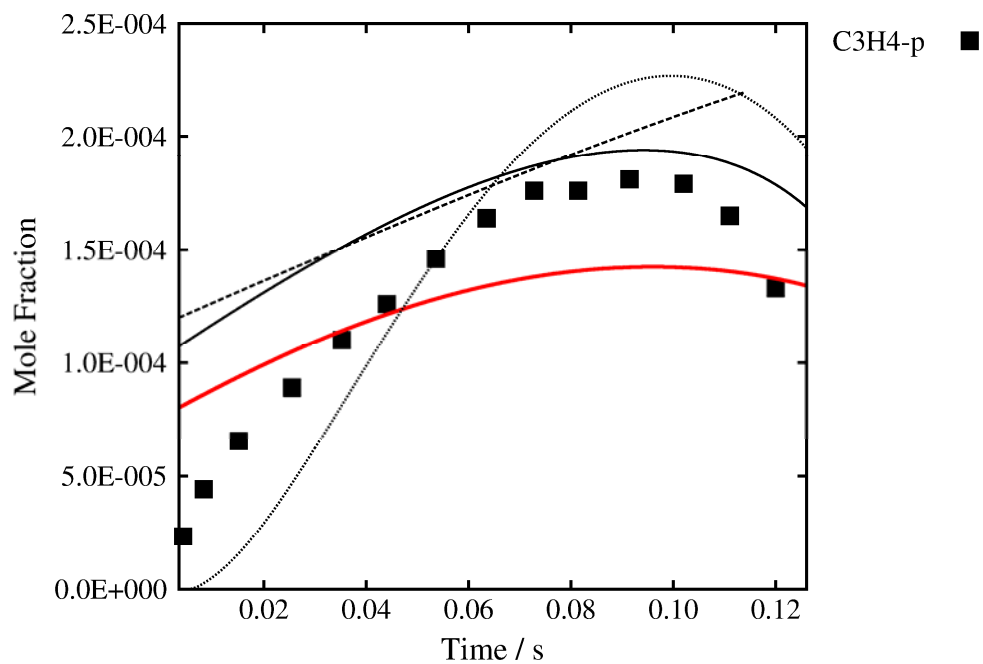
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



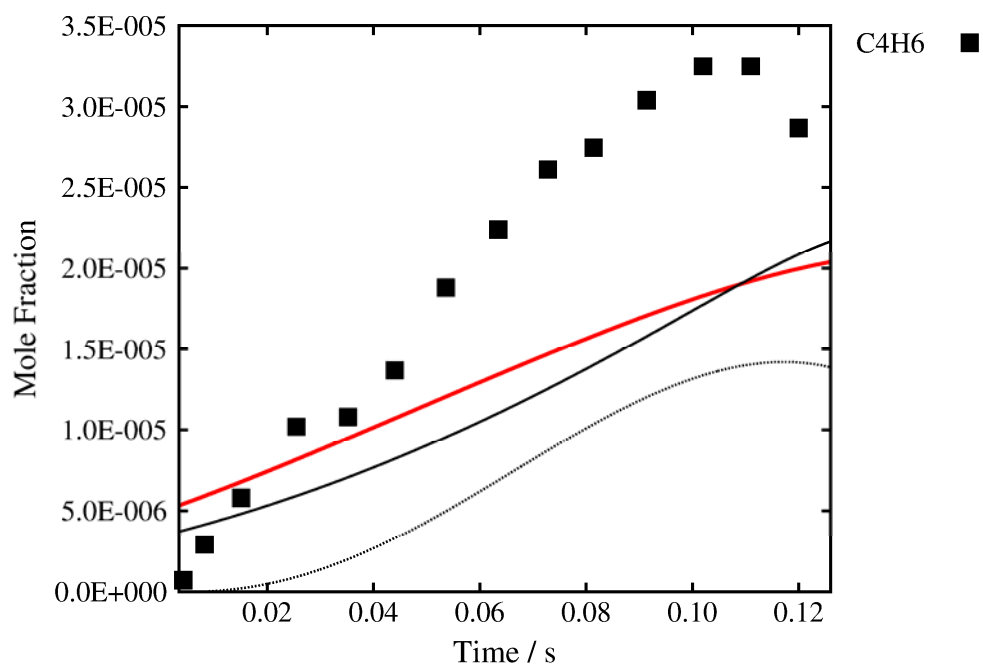
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



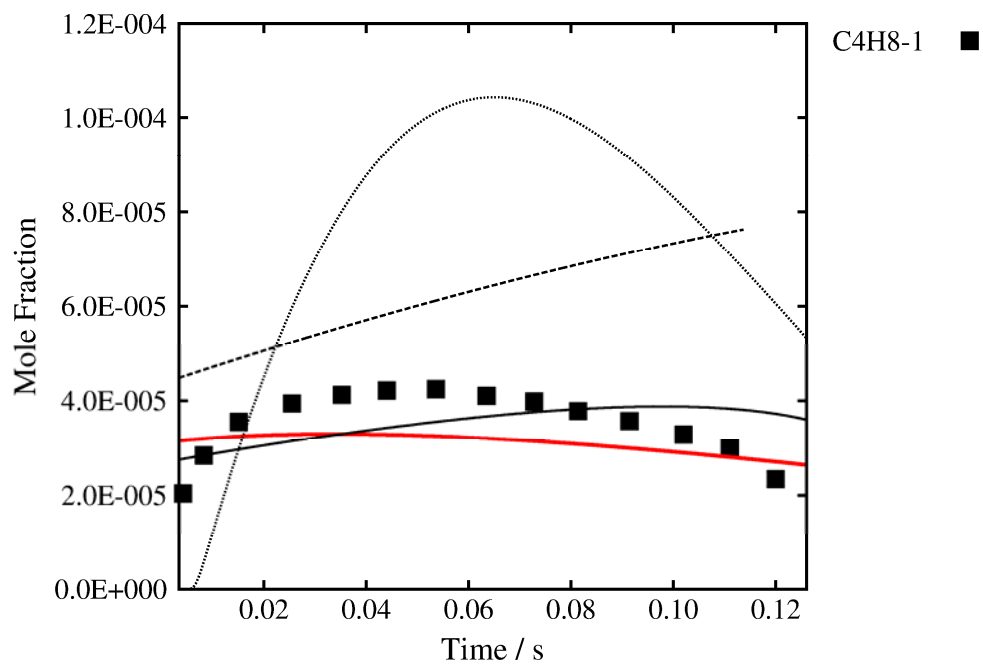
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



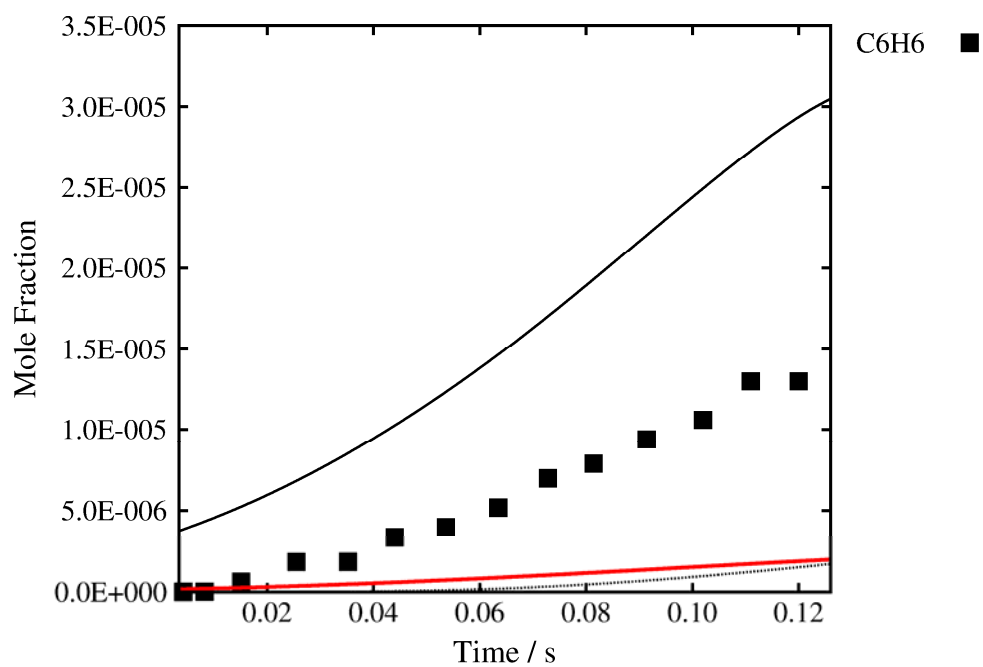
0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K



0.30% C₃H₆ 1.95% O₂ in N₂, $\Phi = 0.70$, $p = 1.0$ atm, $T = 1170$ K

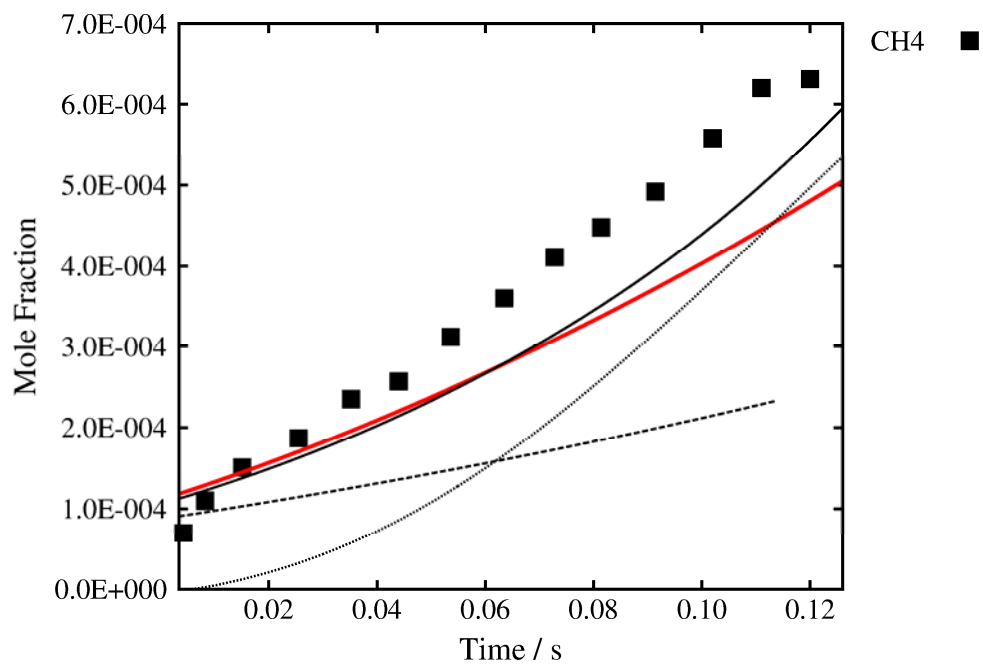
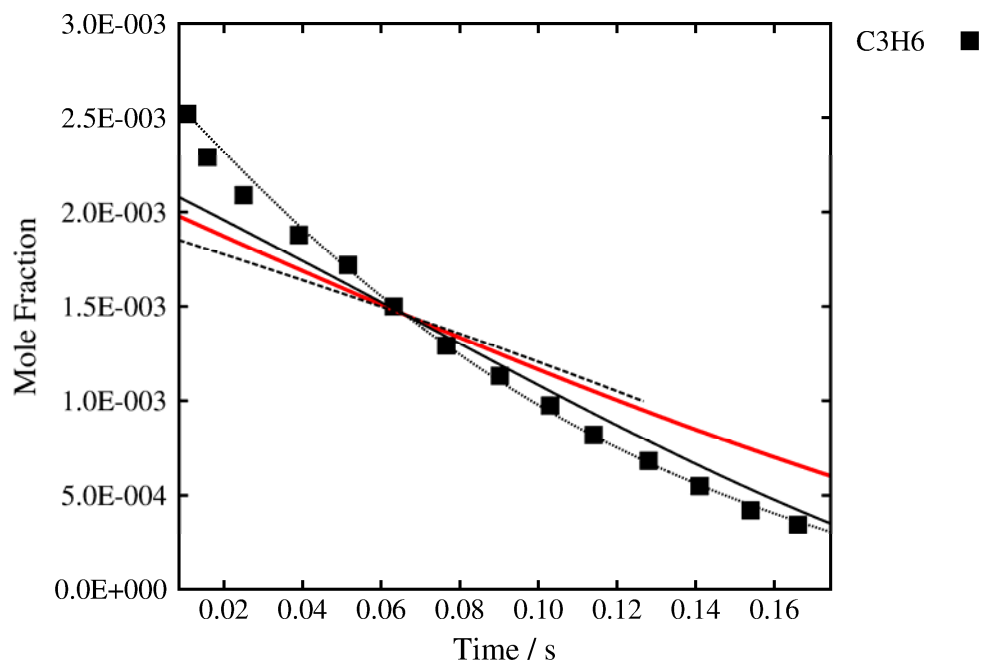
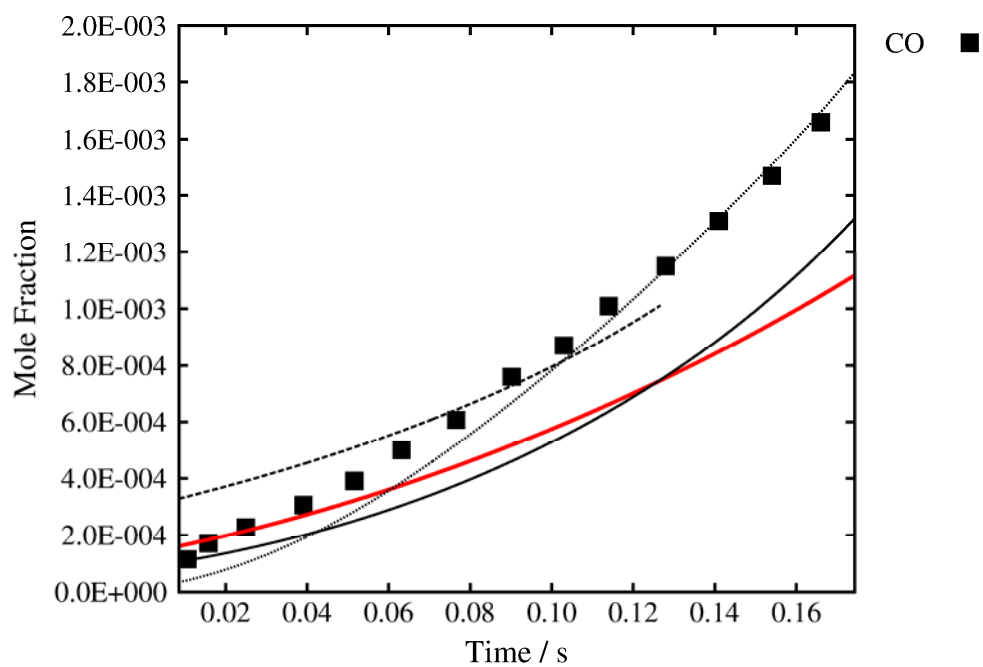


Figure 18 Flow times of propene/O₂/N₂. Symbols are experimental data [3] lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

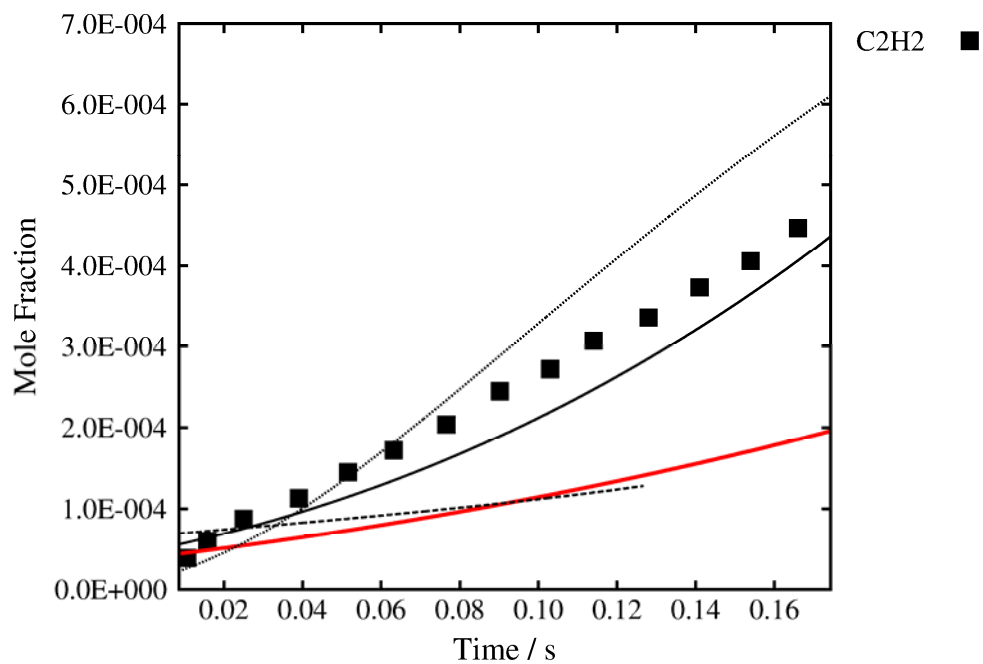
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



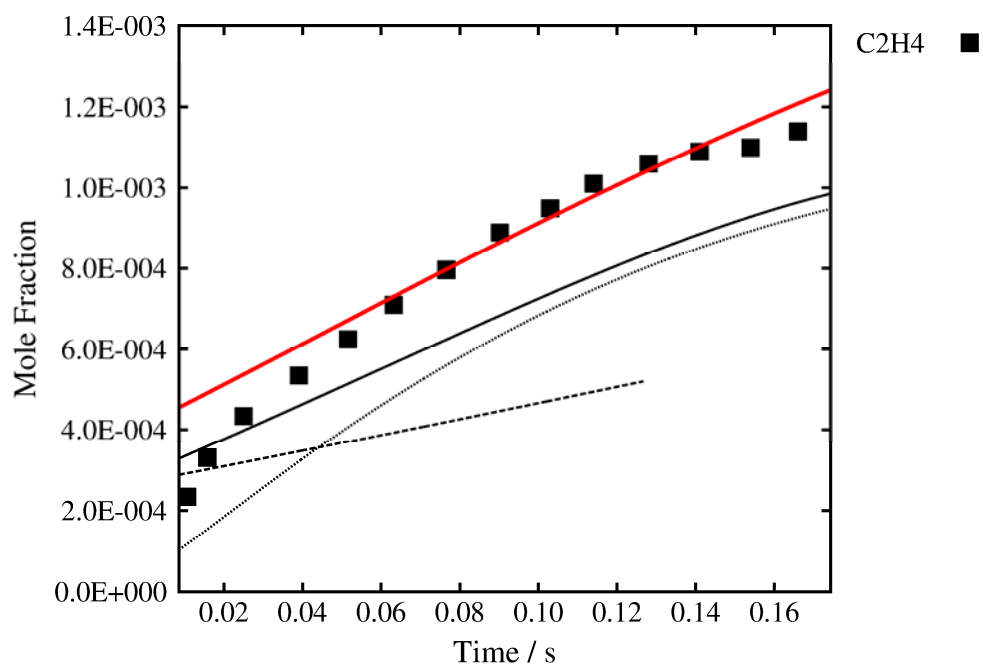
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



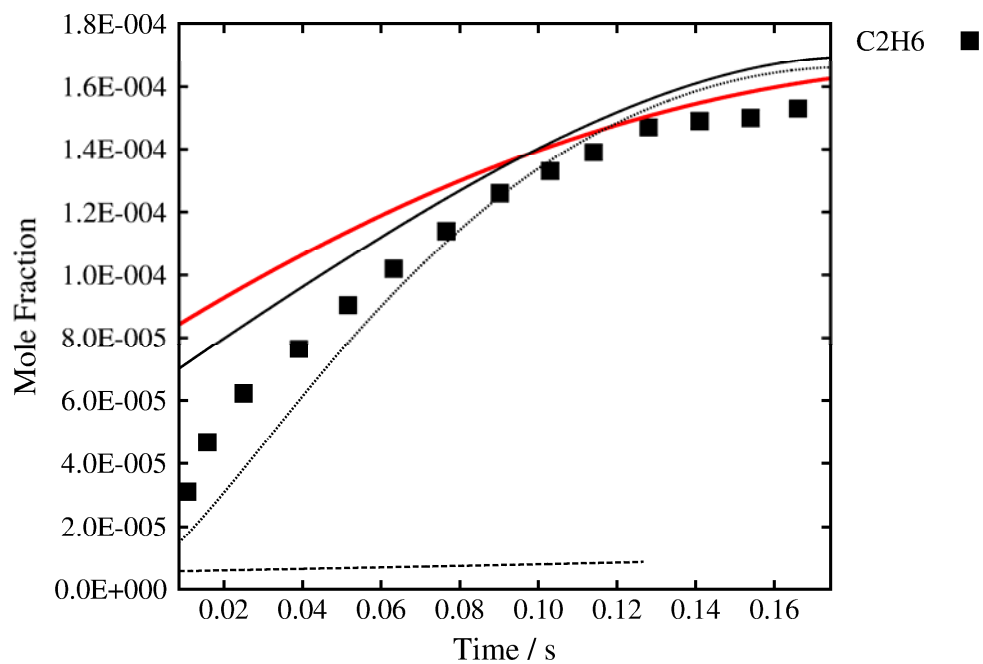
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



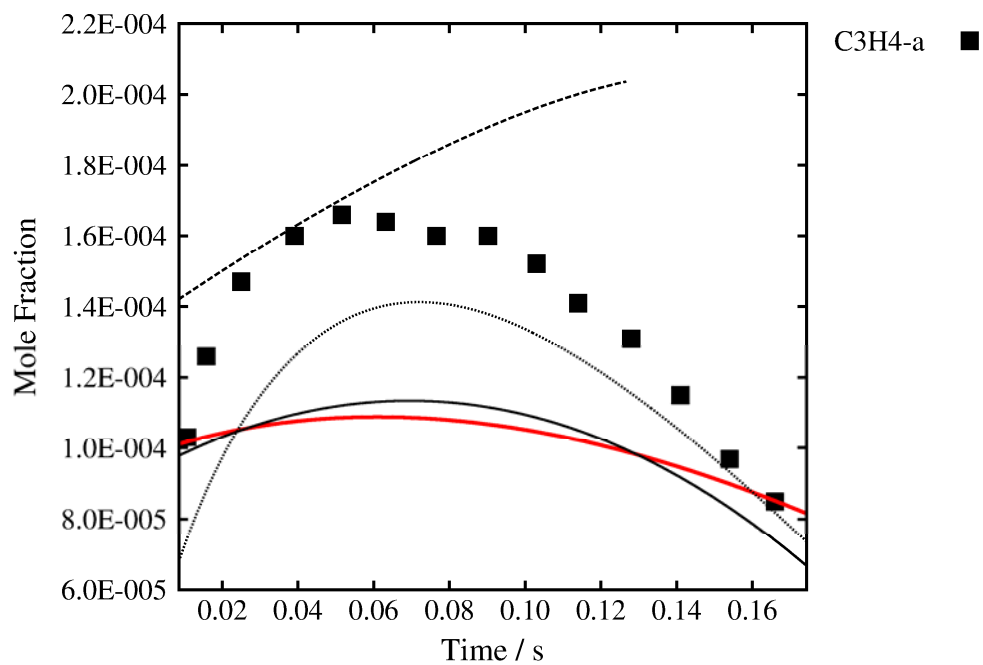
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



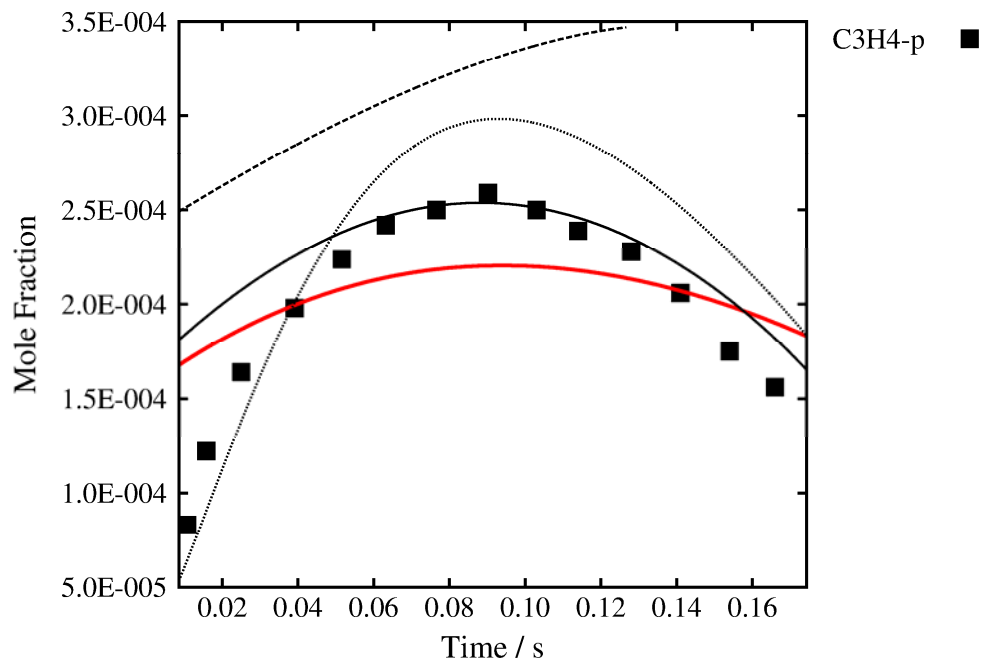
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



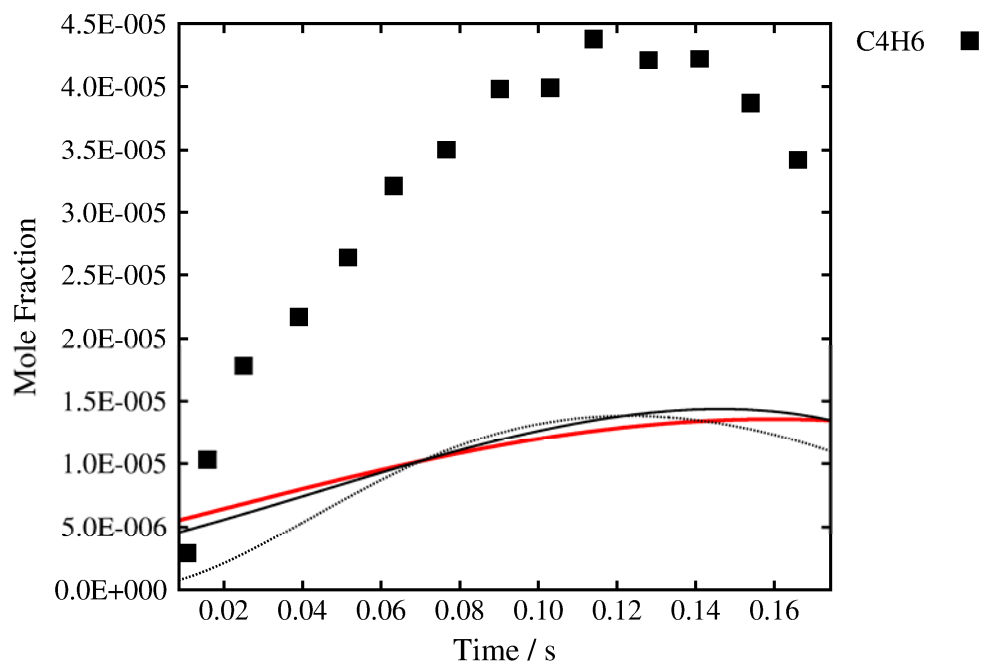
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



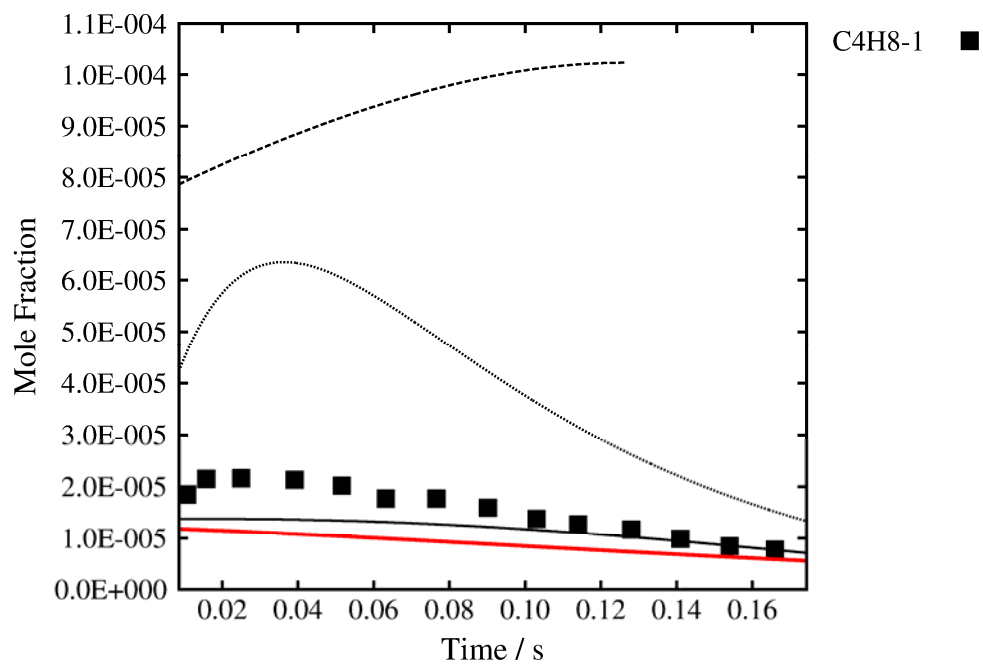
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



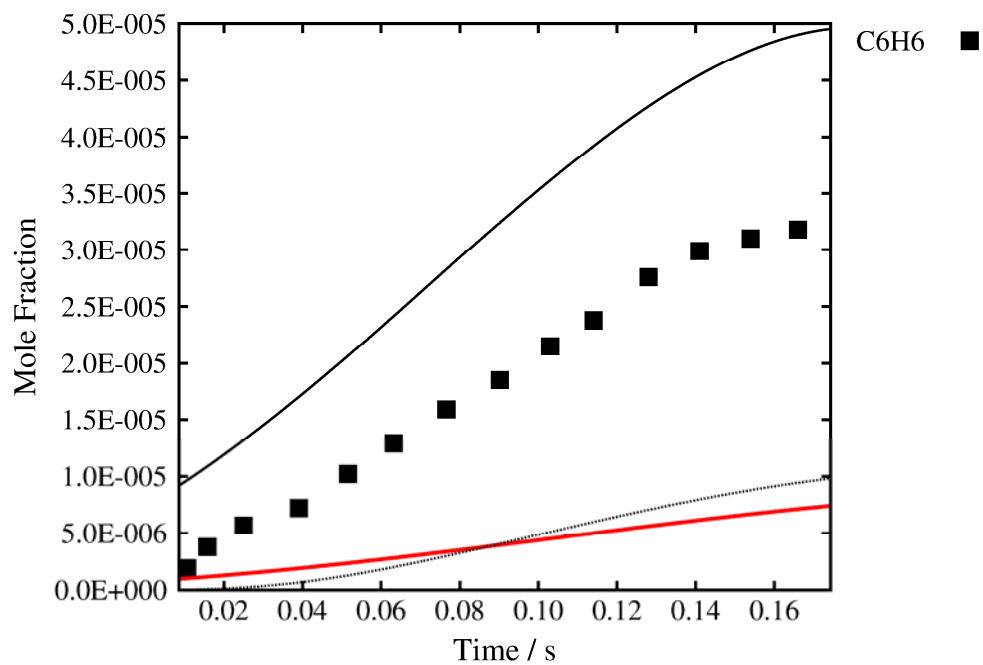
0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K



0.29% C₃H₆ 0.92% O₂ in N₂, $\Phi = 1.42$, $p = 1.0$ atm, $T = 1200$ K

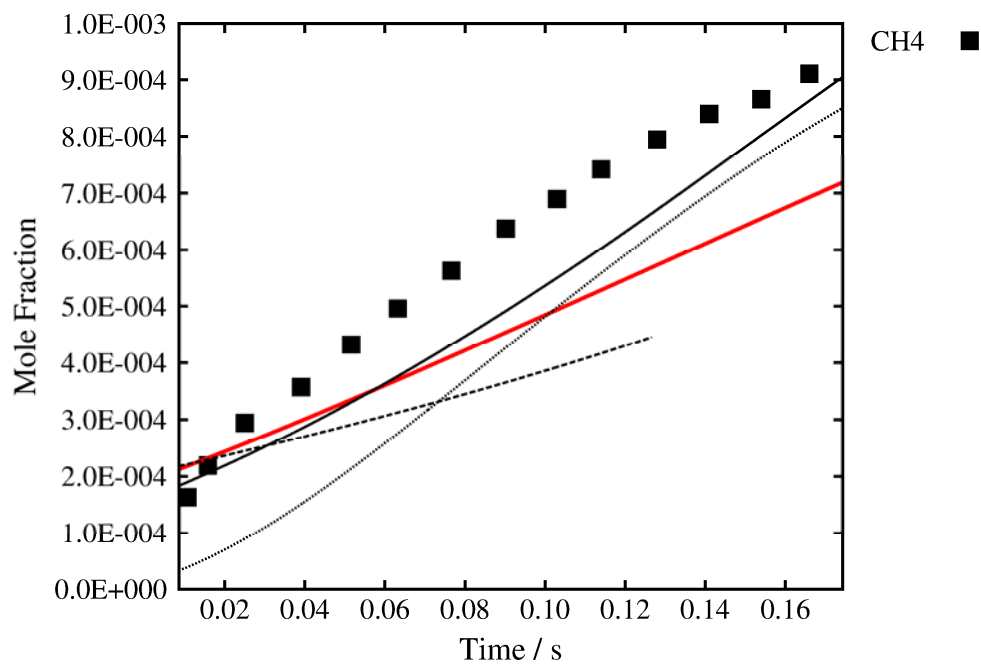
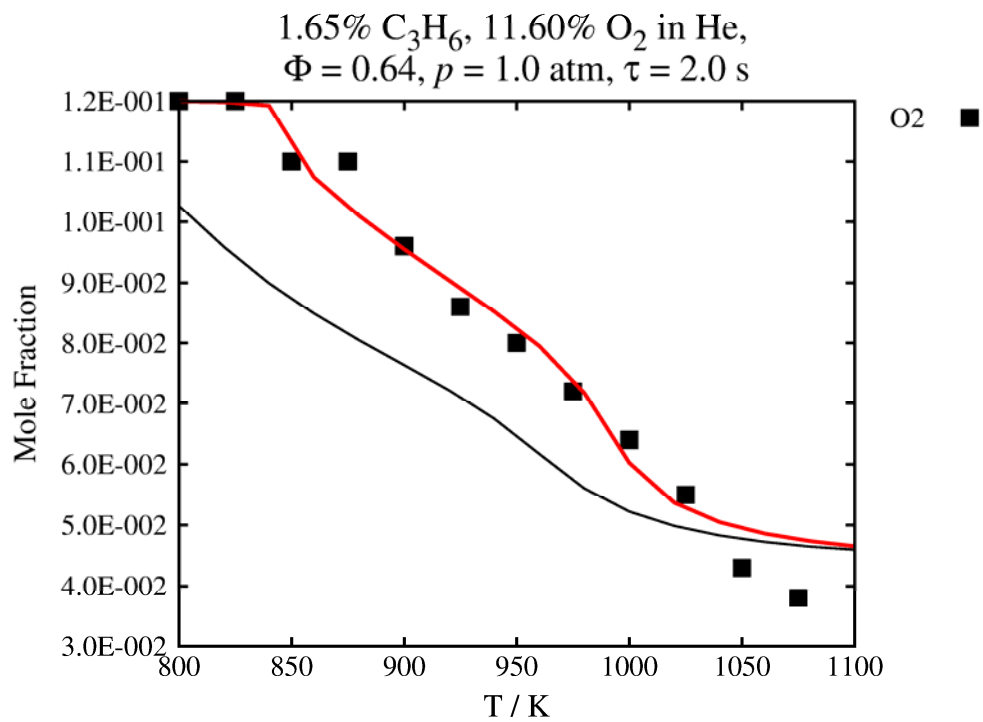
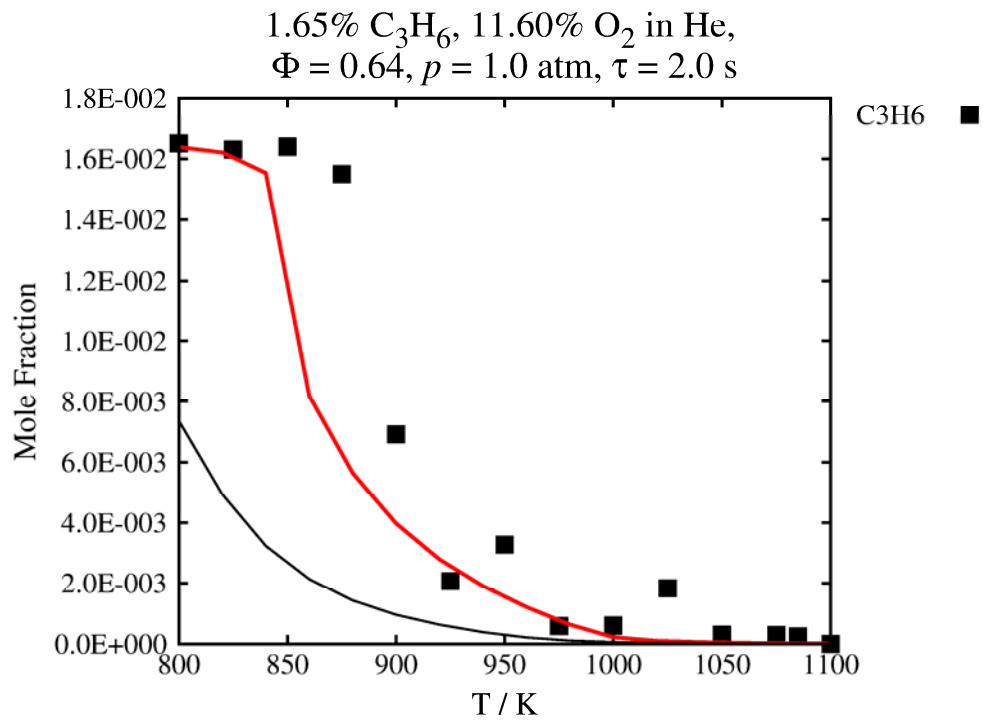
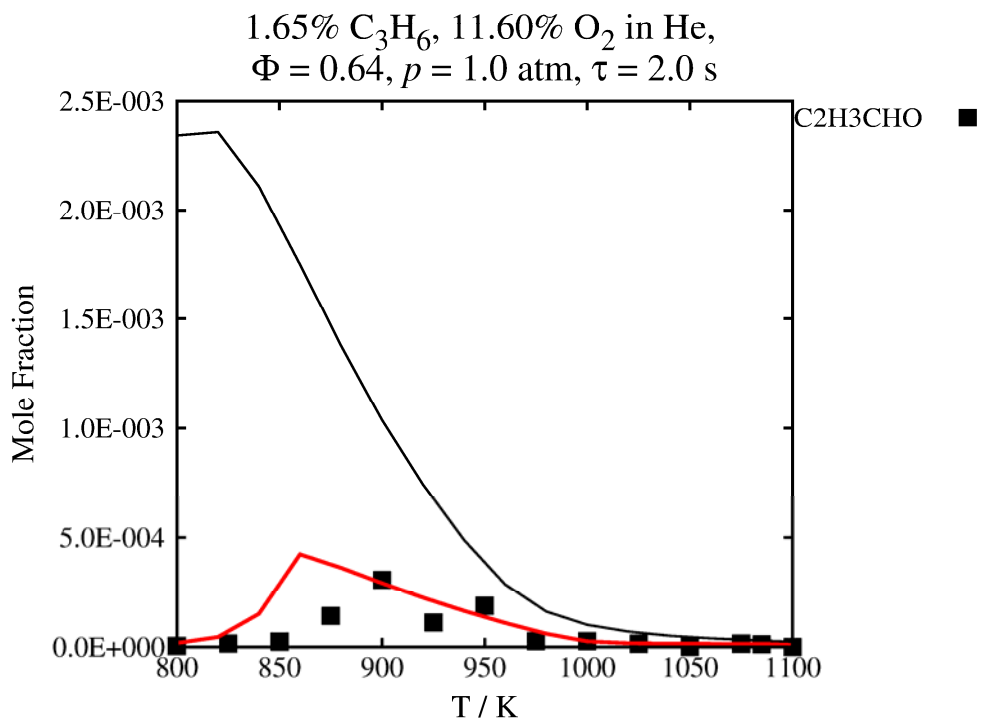
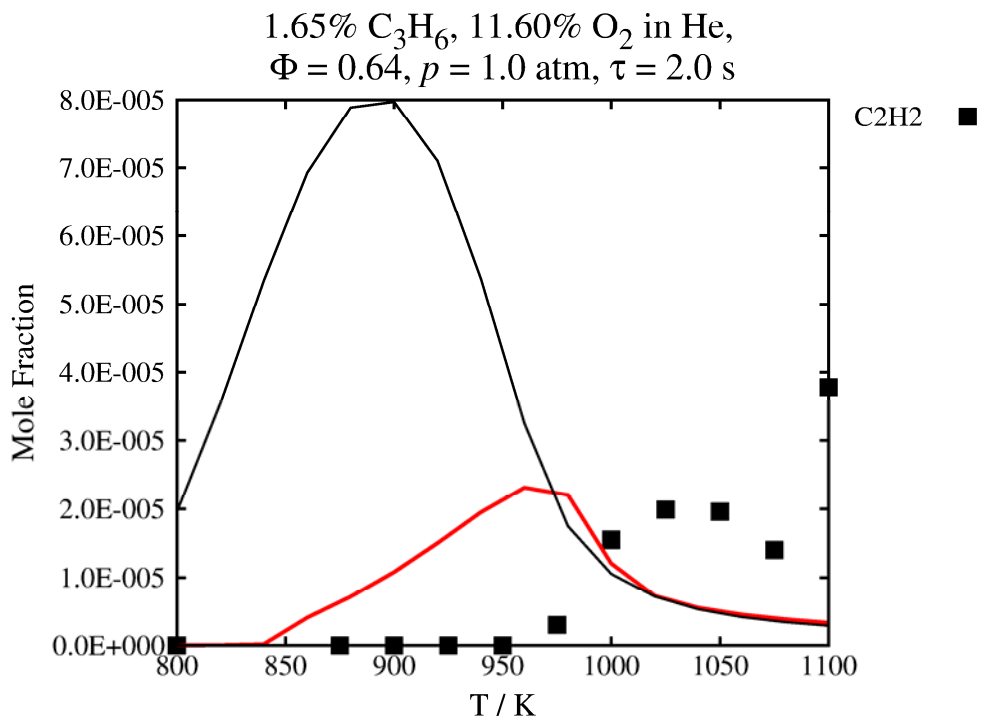


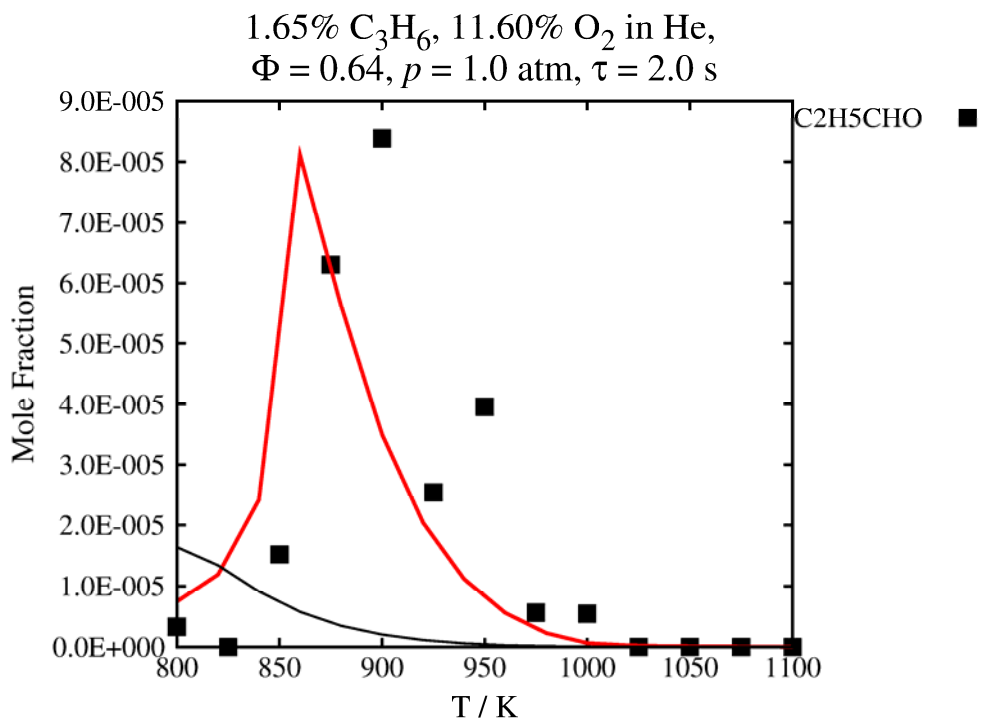
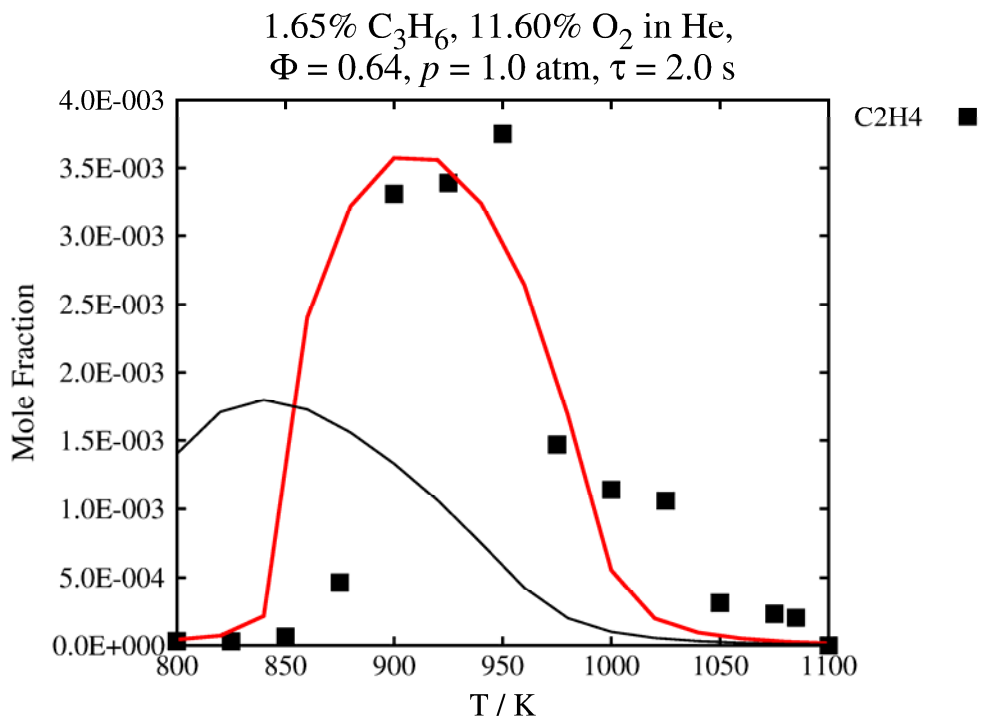
Figure 19 Flow times of propene/O₂/N₂. Symbols are experimental data [3] lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

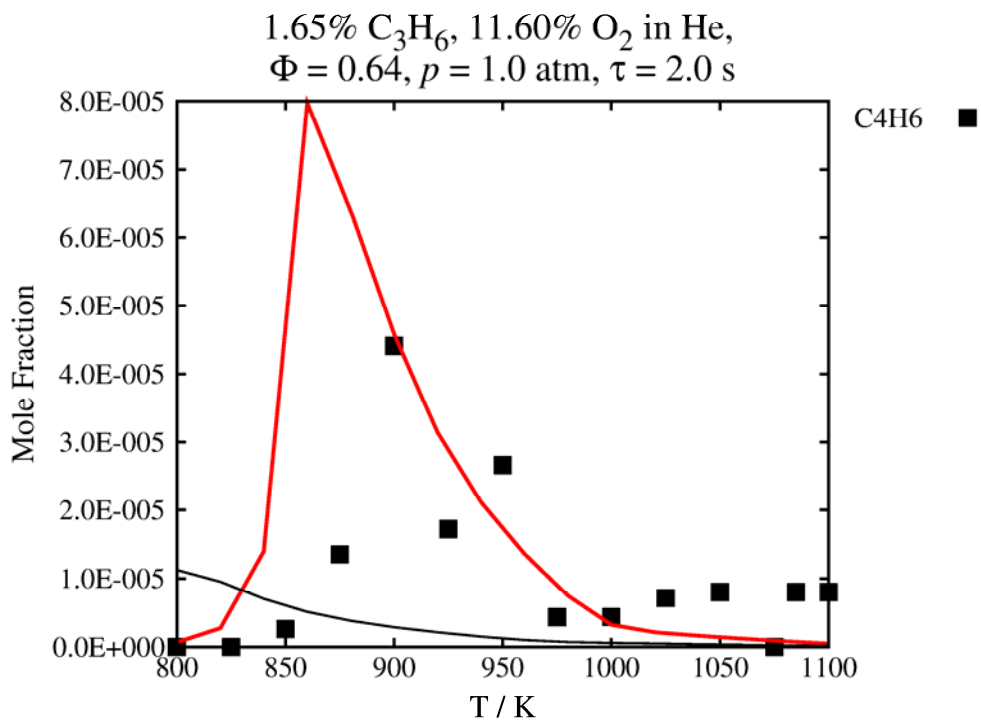
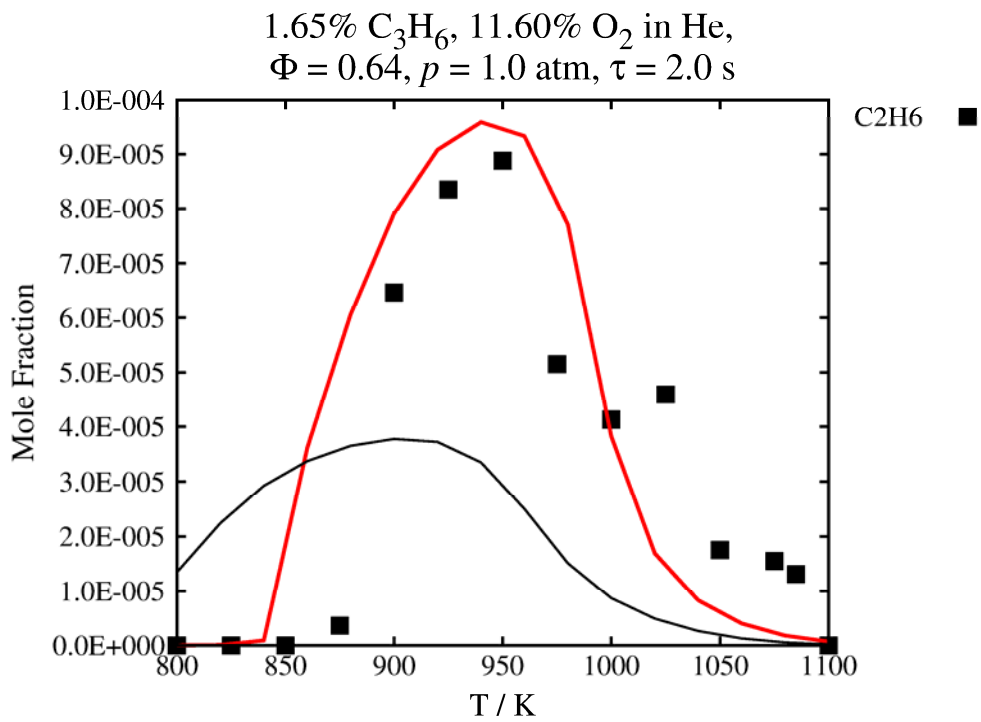
Targets from Part I and II of this study

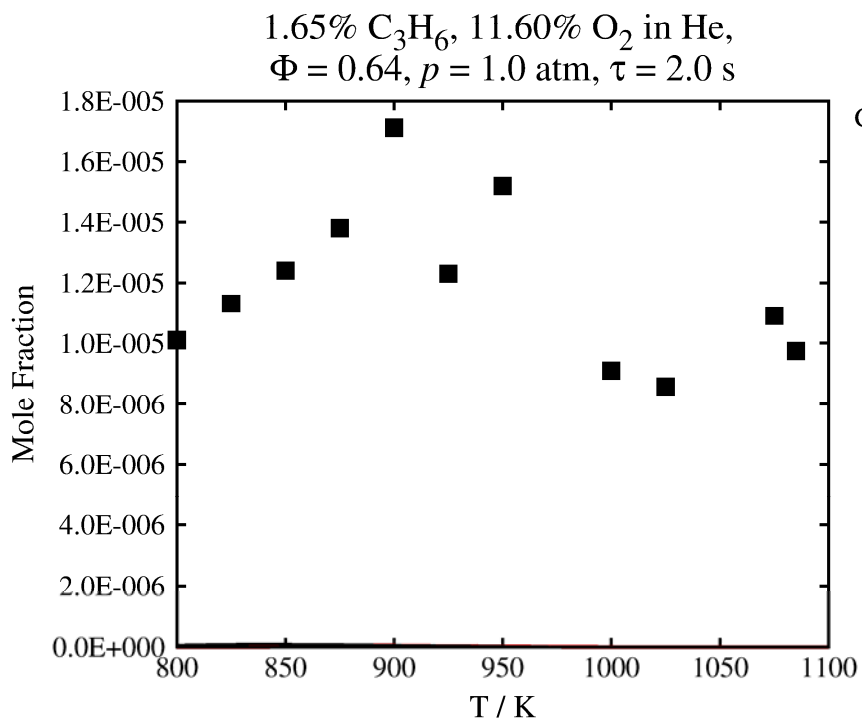
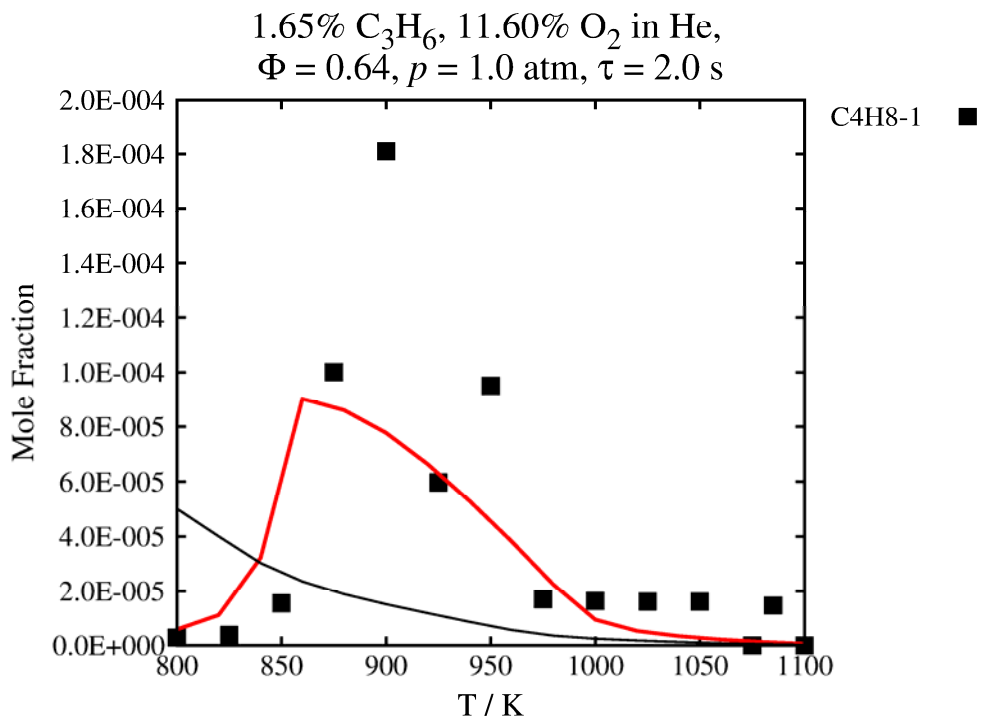
JSR

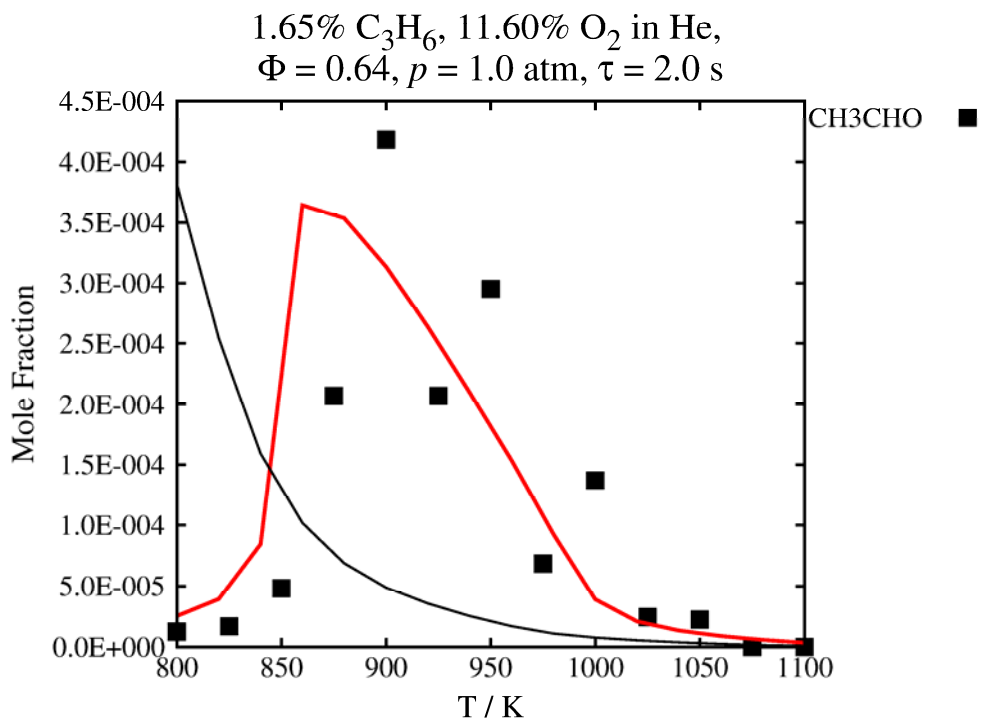
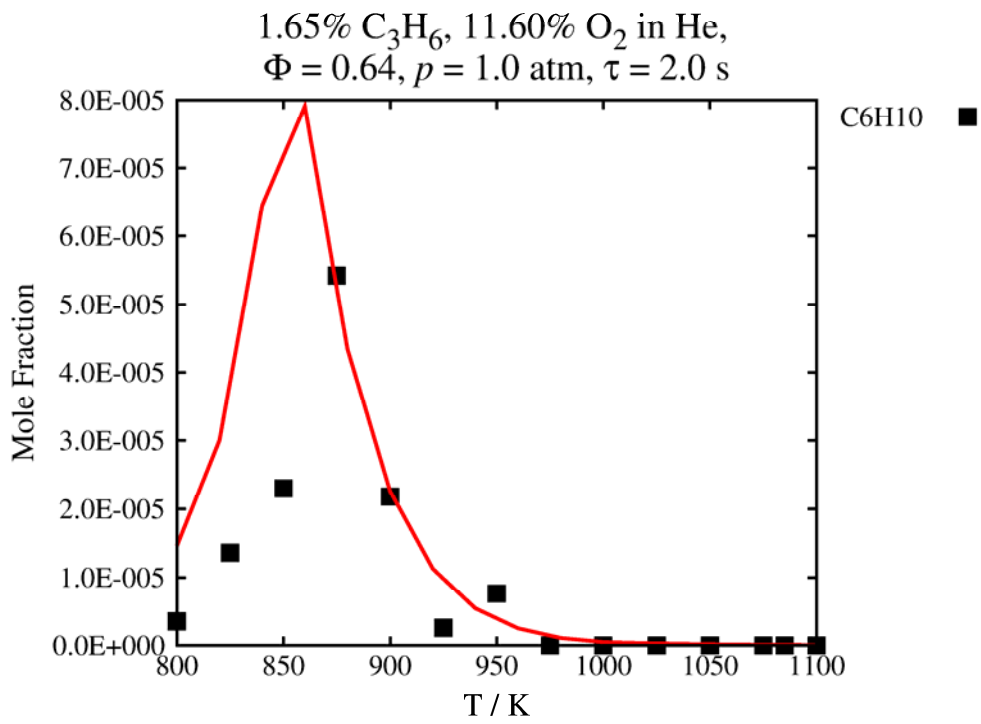


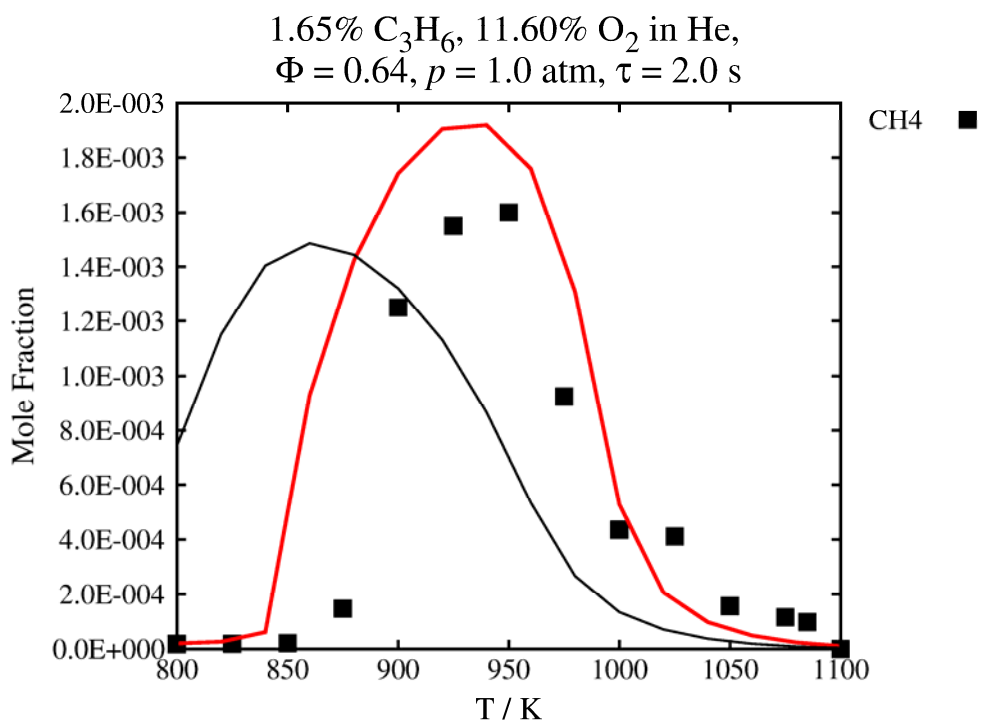
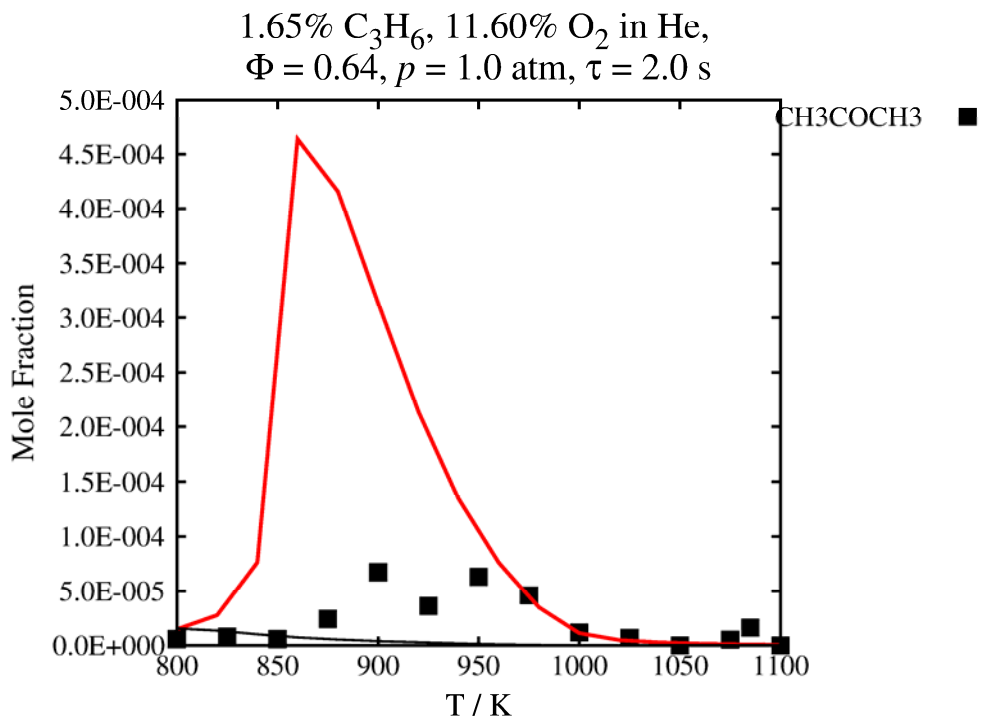












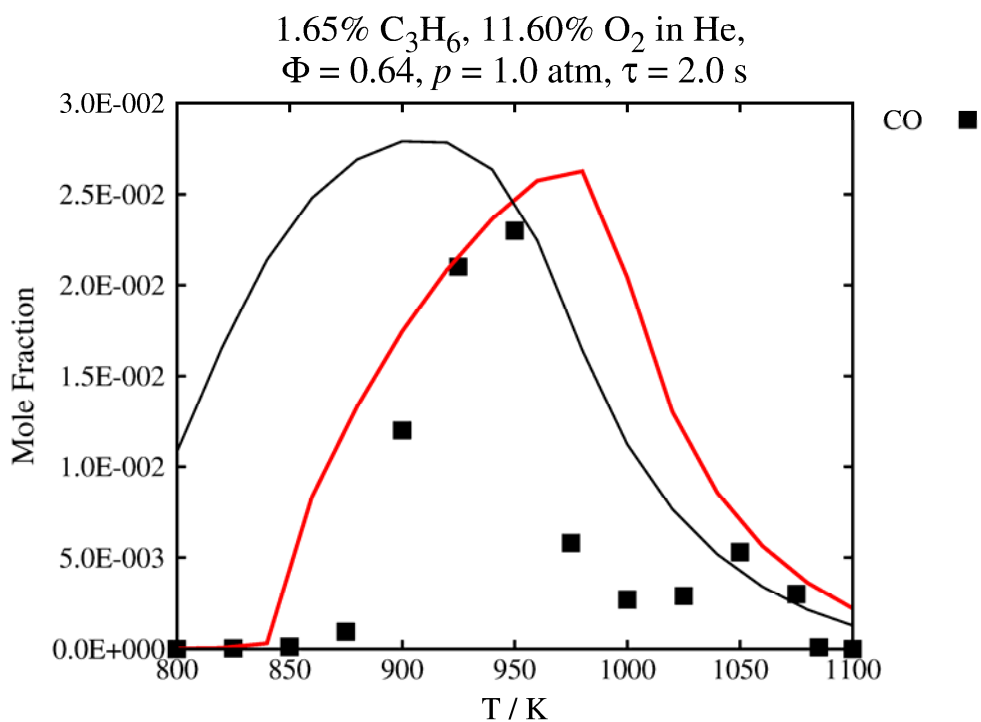
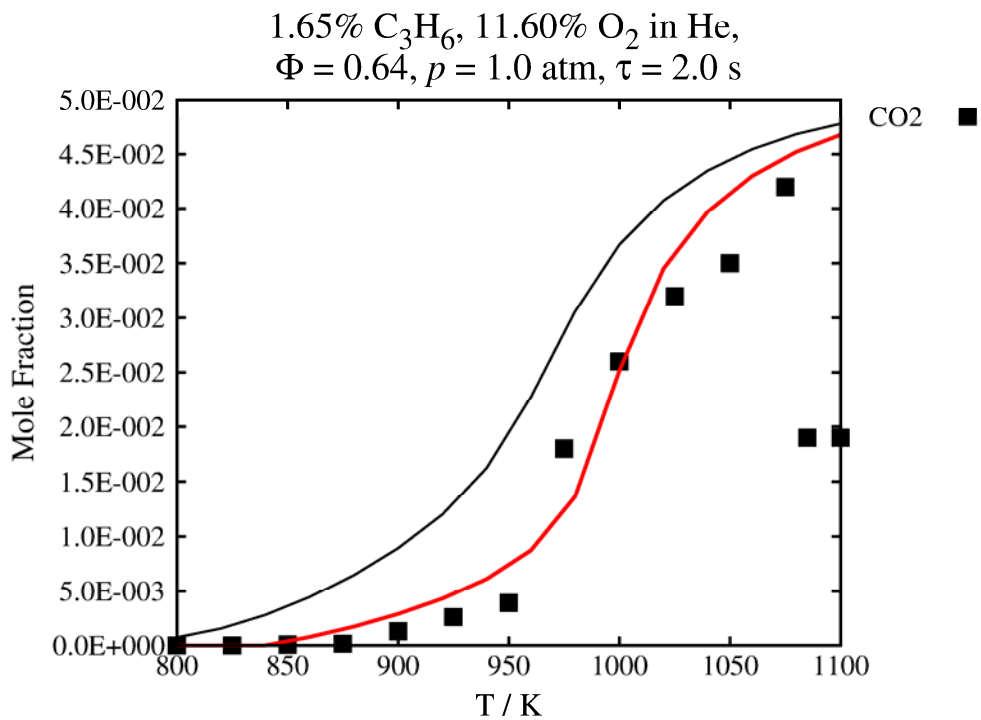
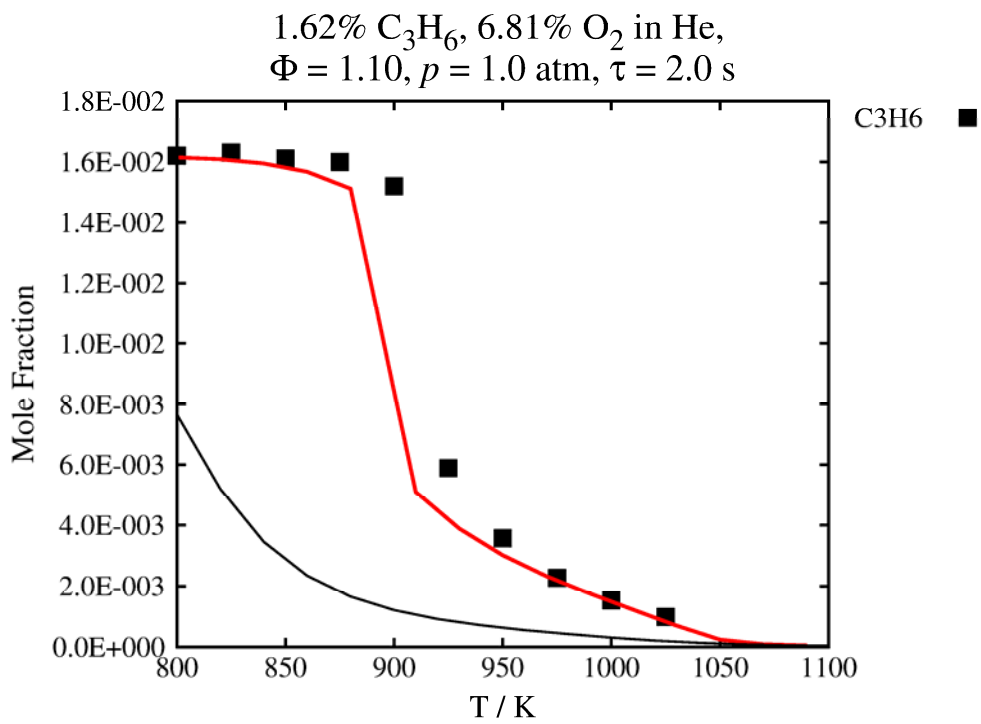
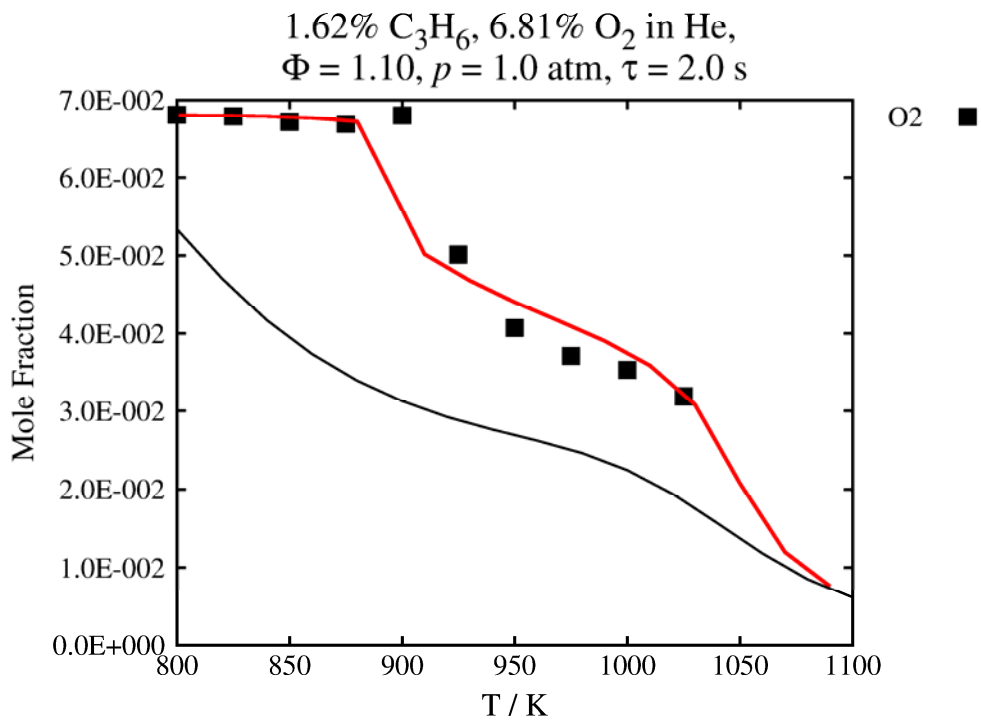
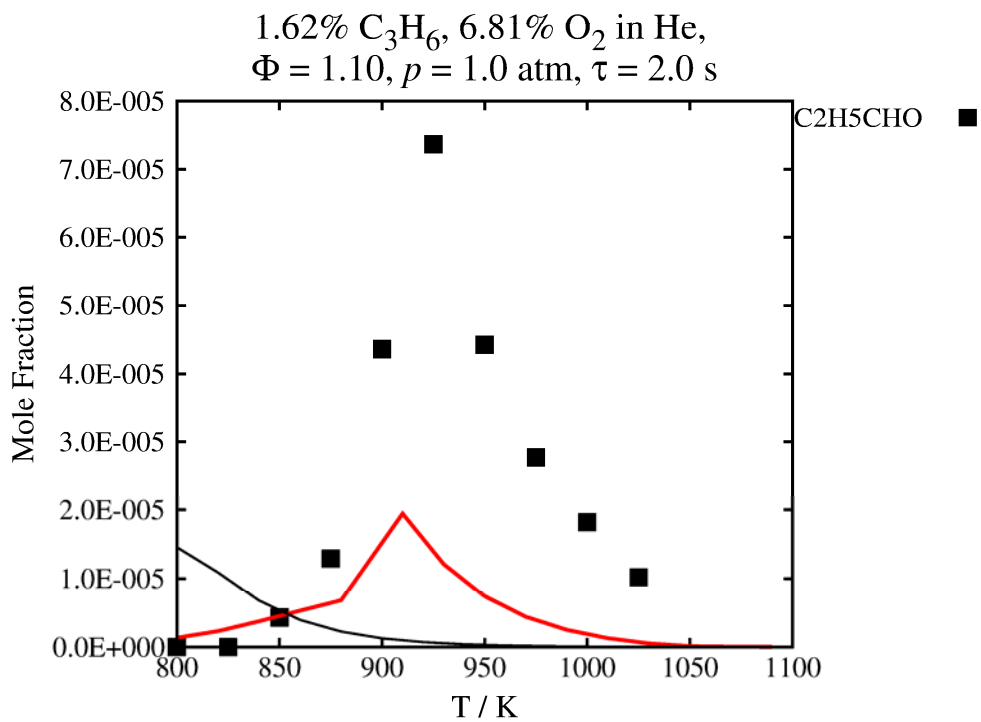
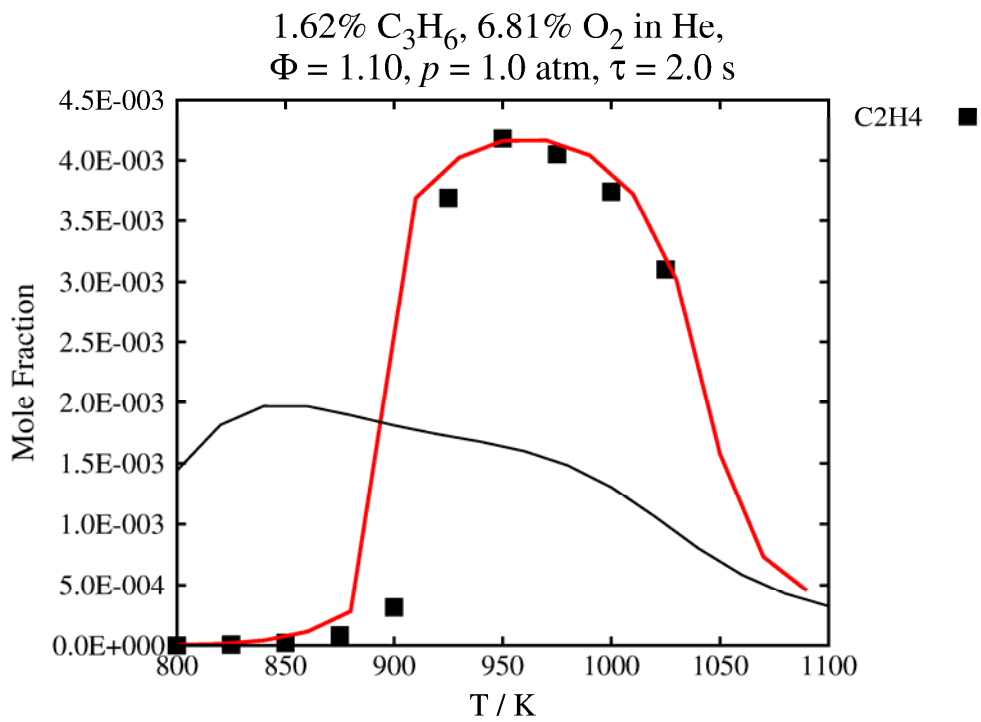
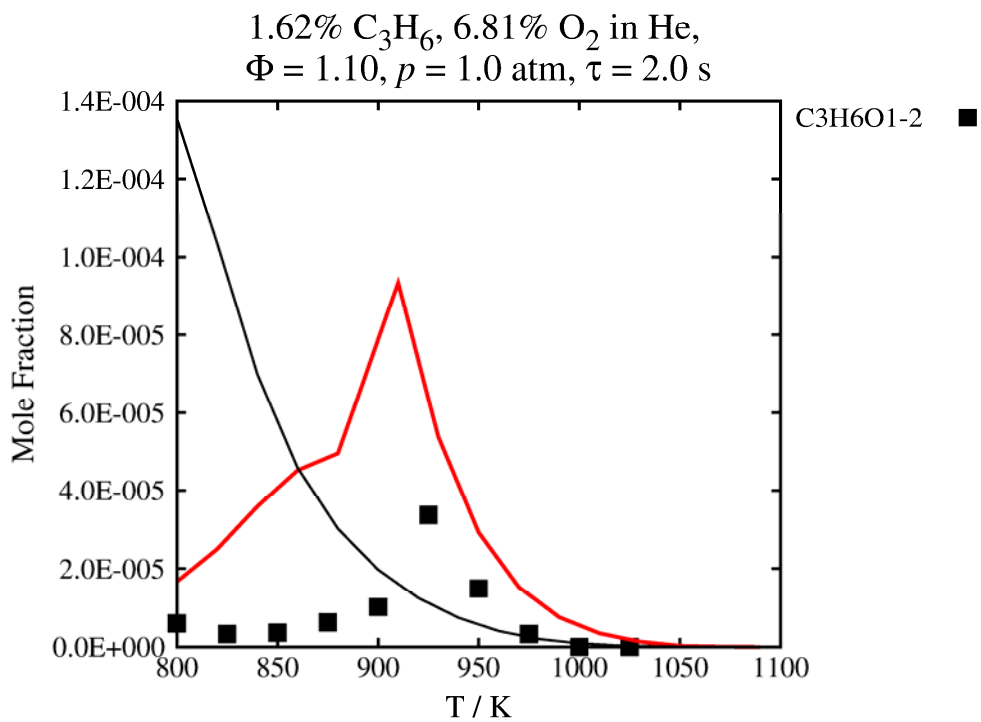
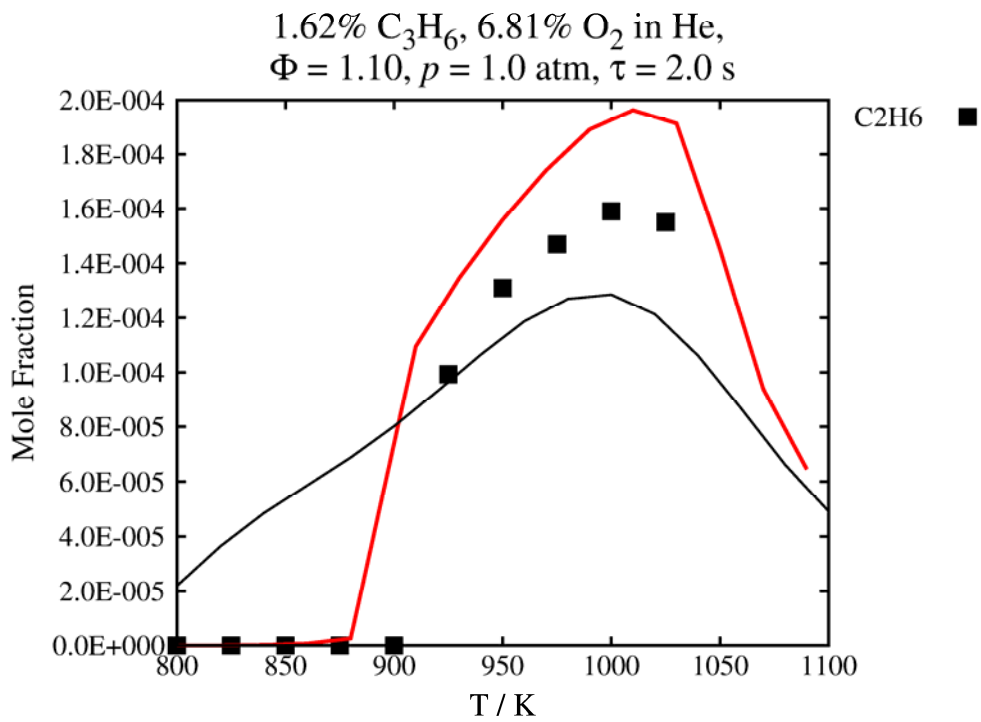
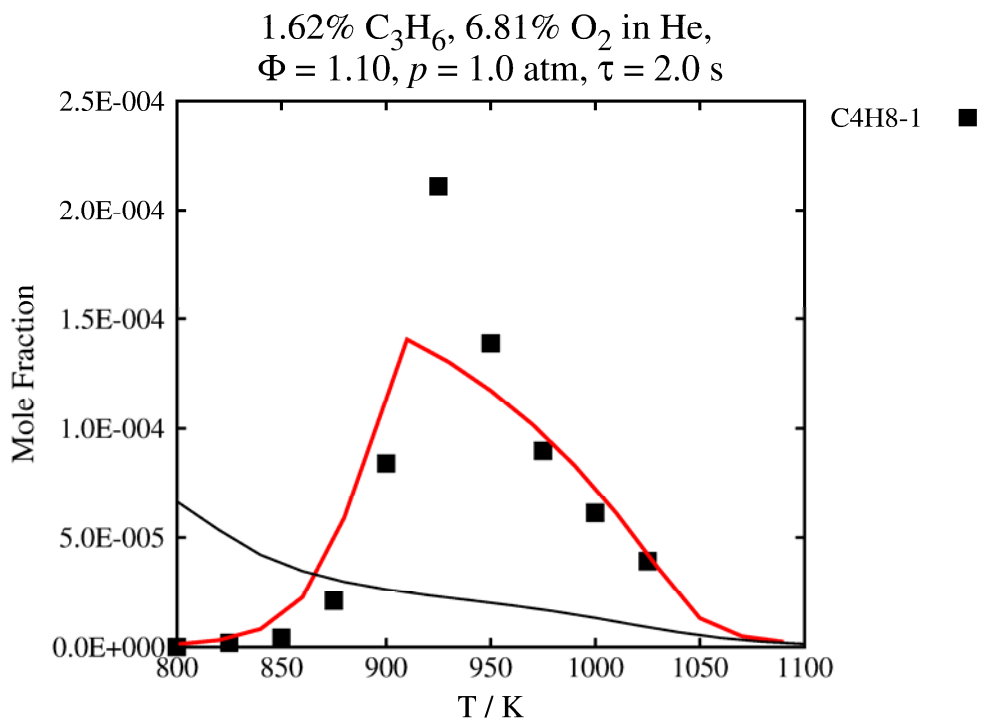
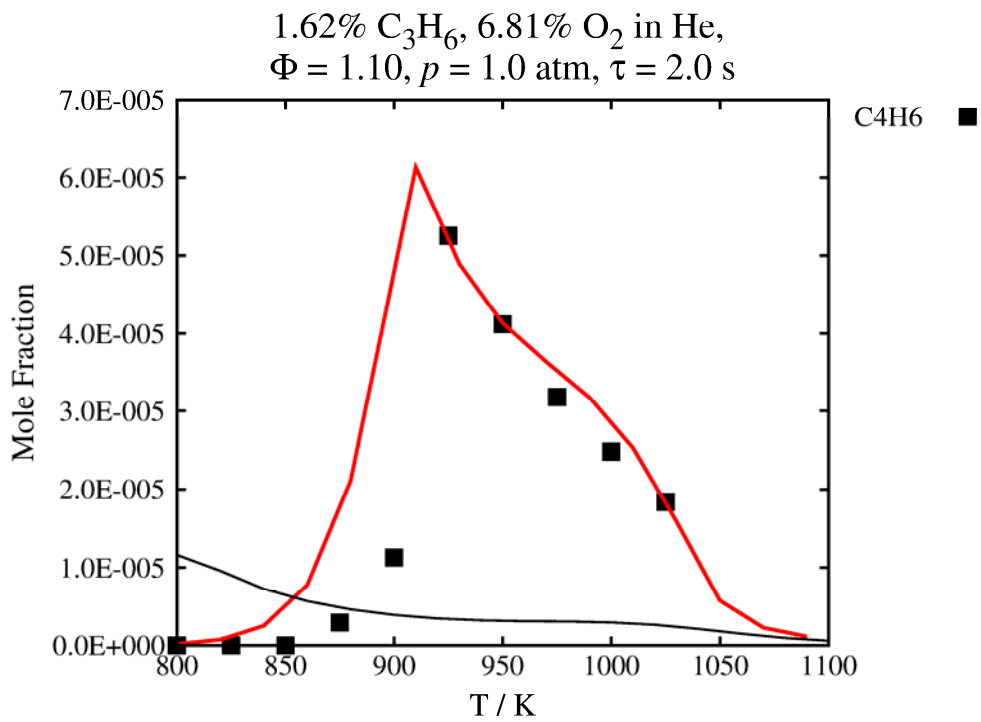


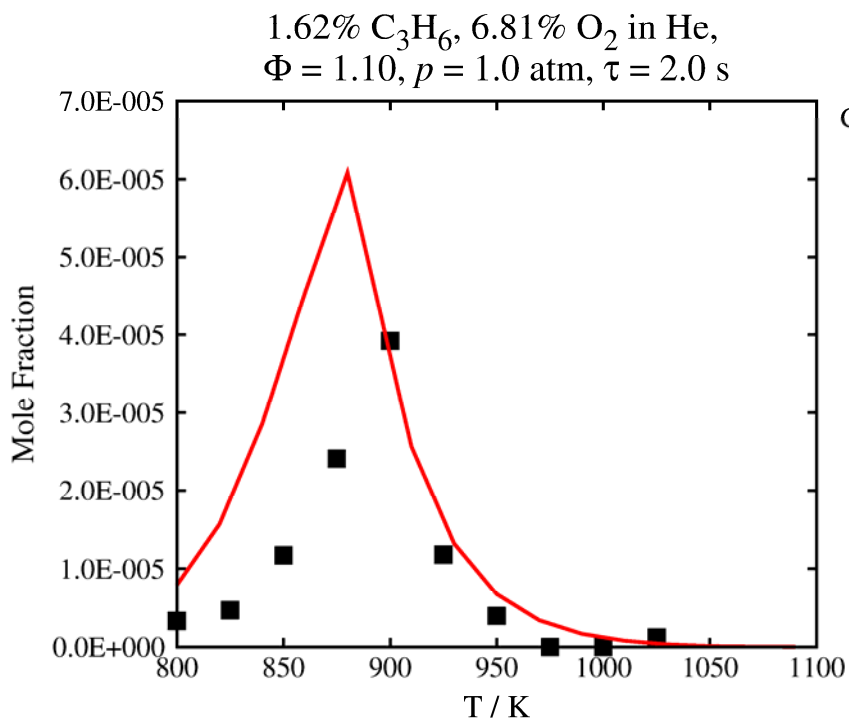
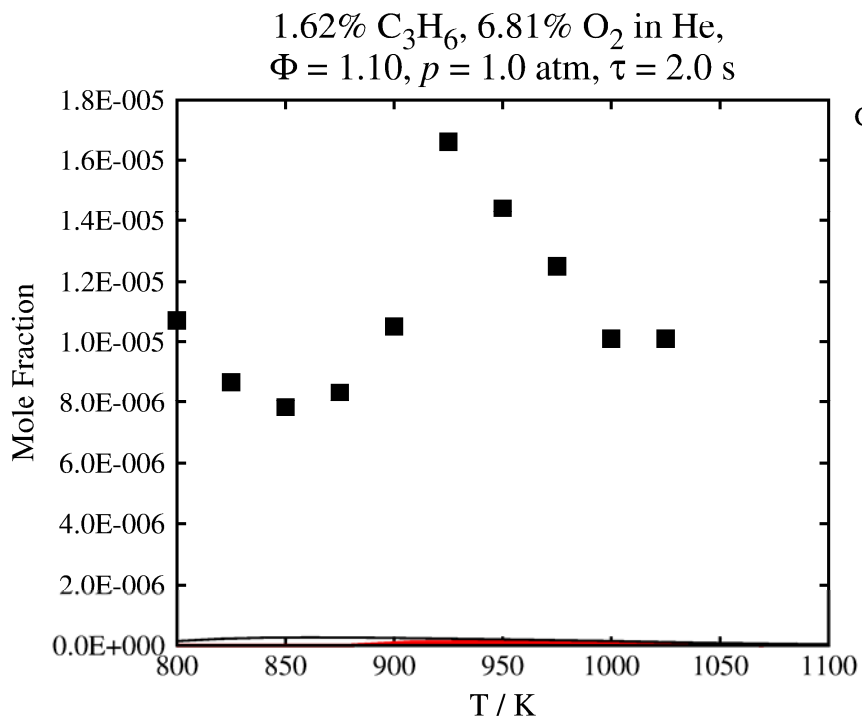
Figure 20 Jet-stirred reactor of propene/O₂/He. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

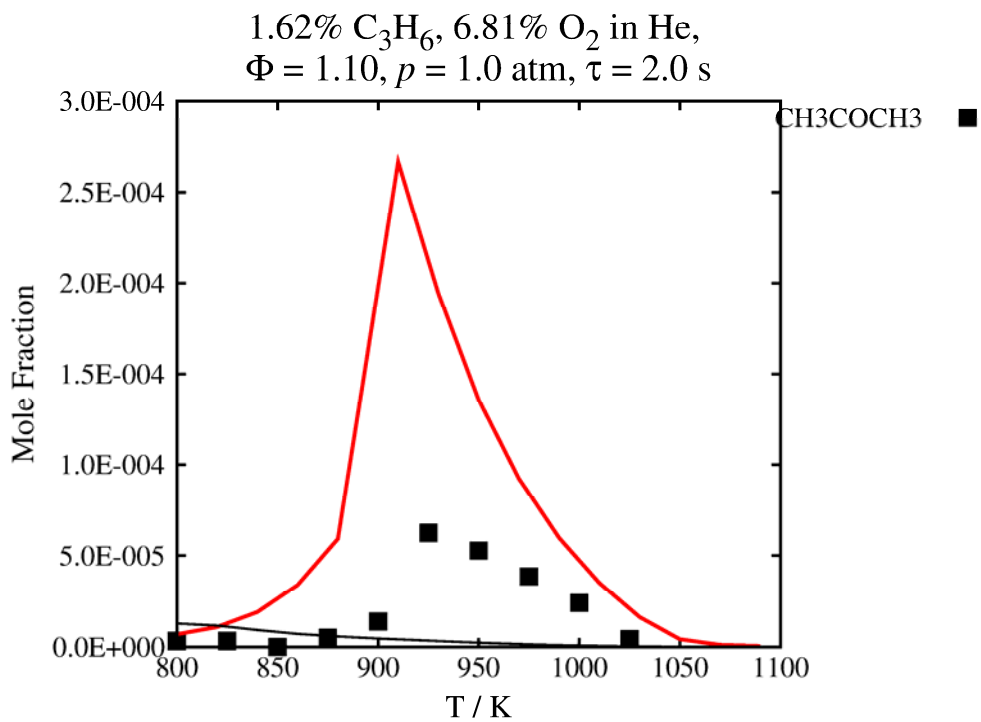
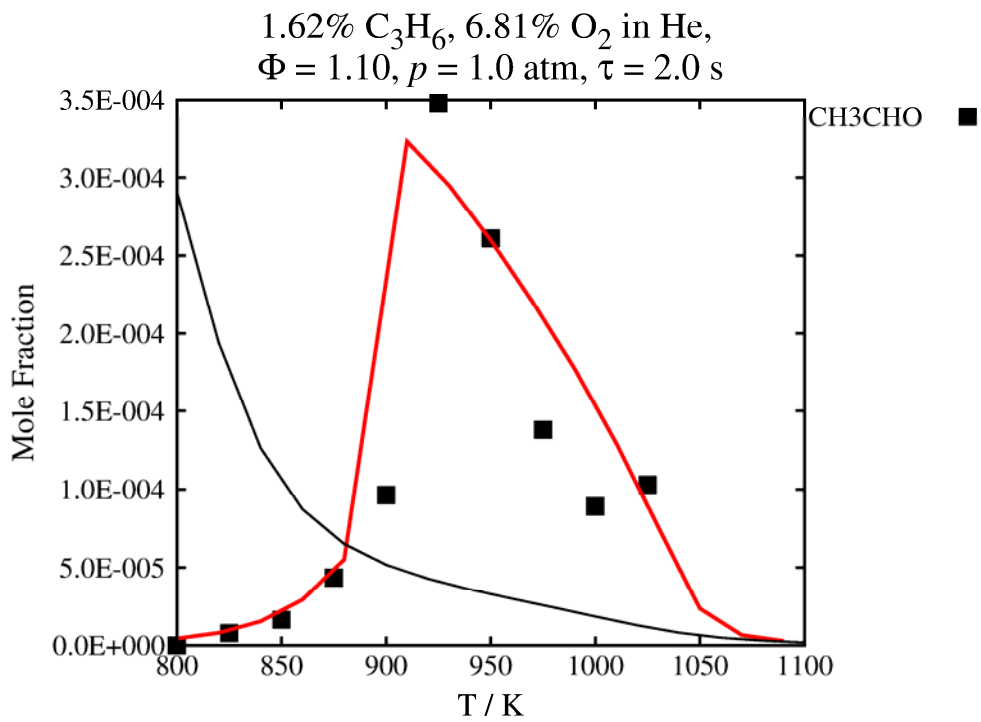


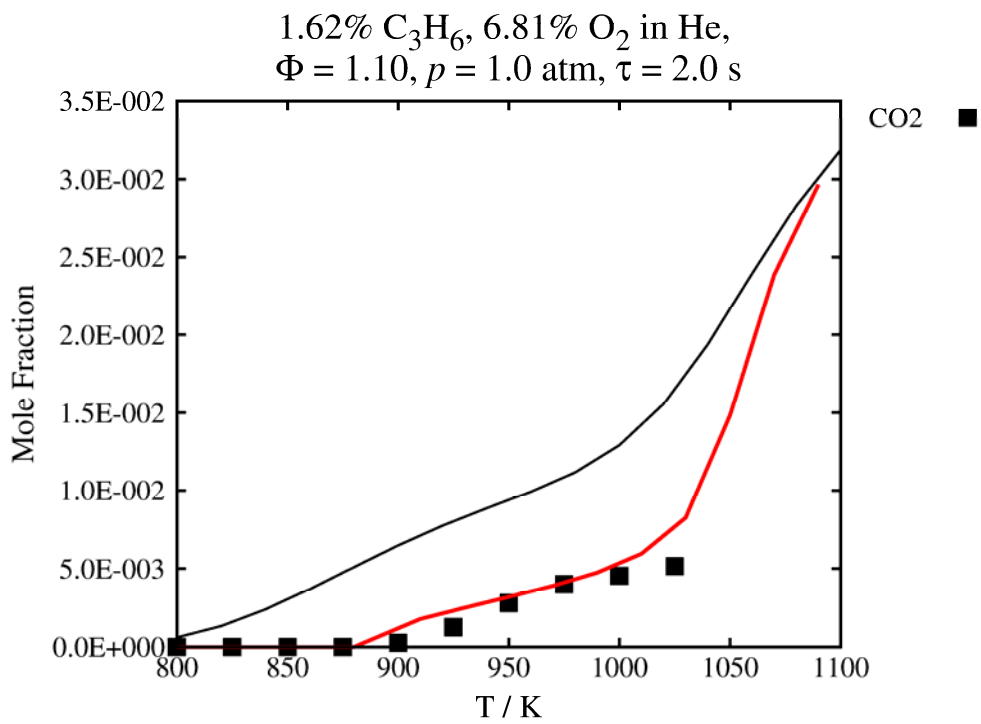
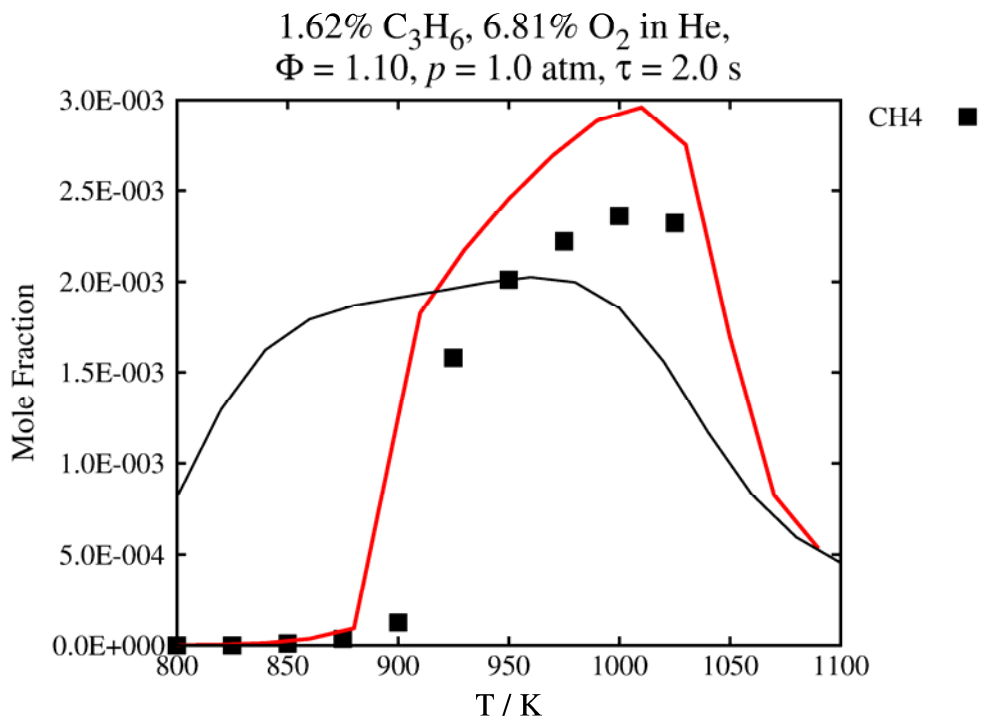












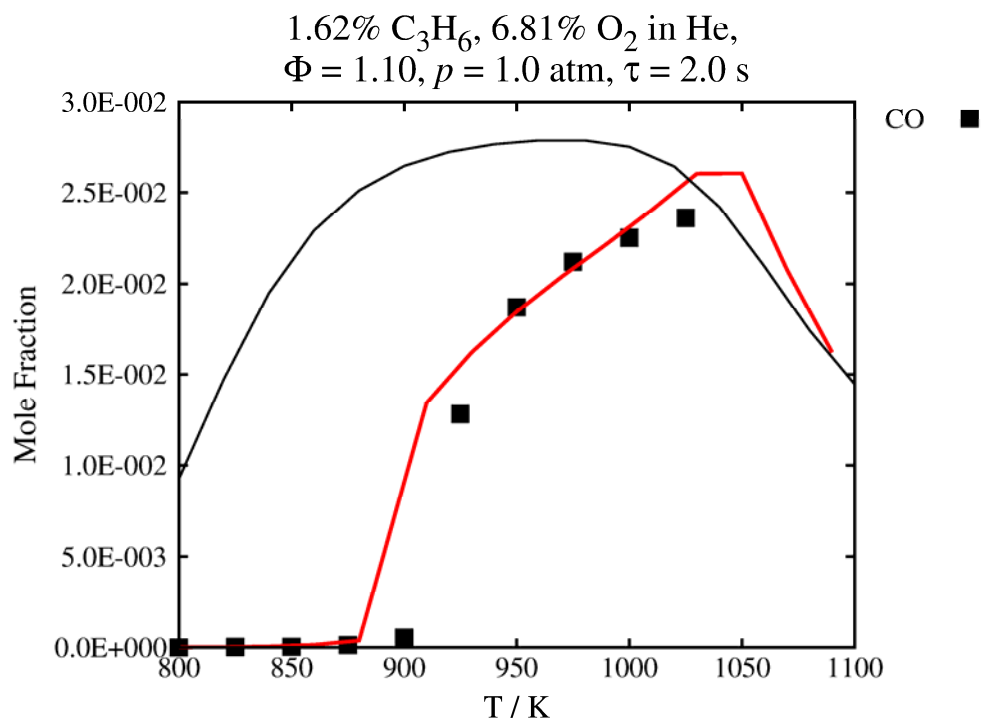
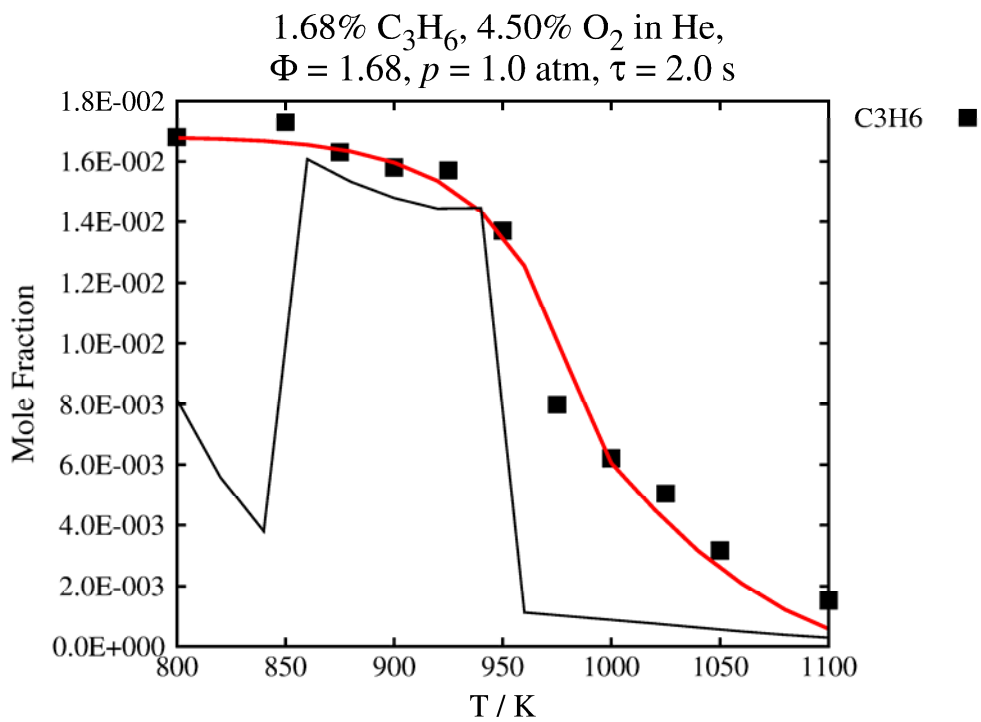
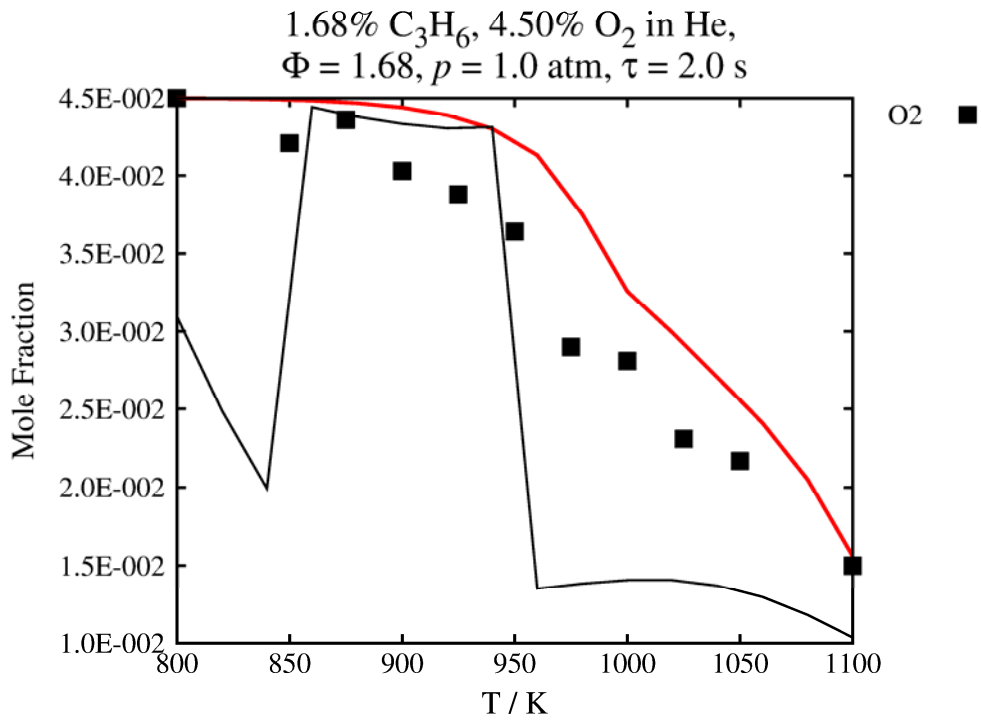
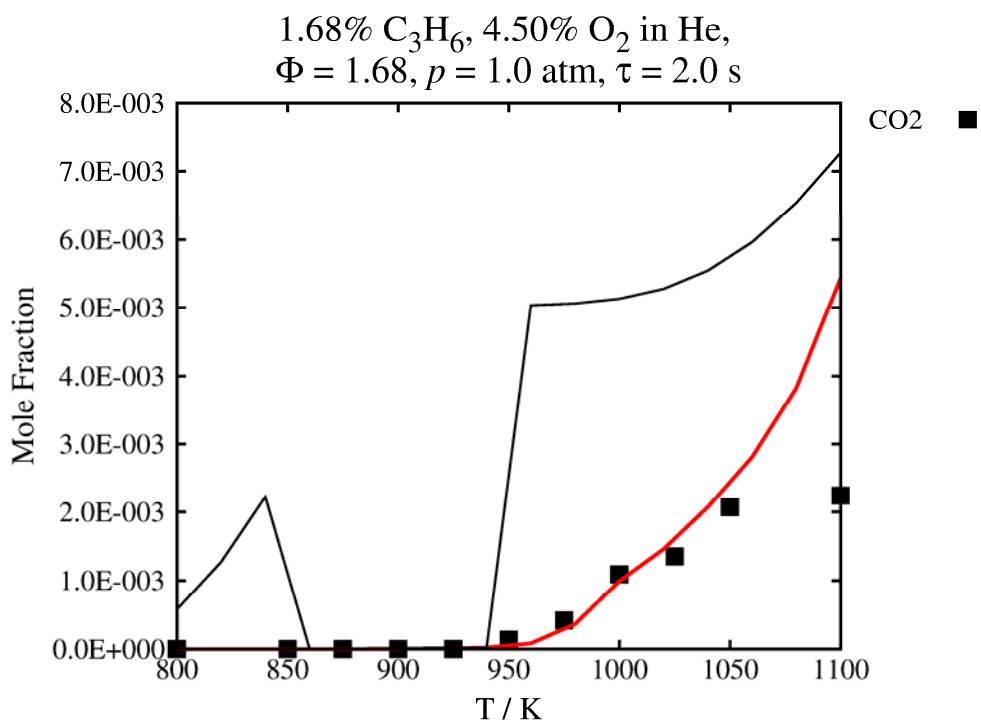
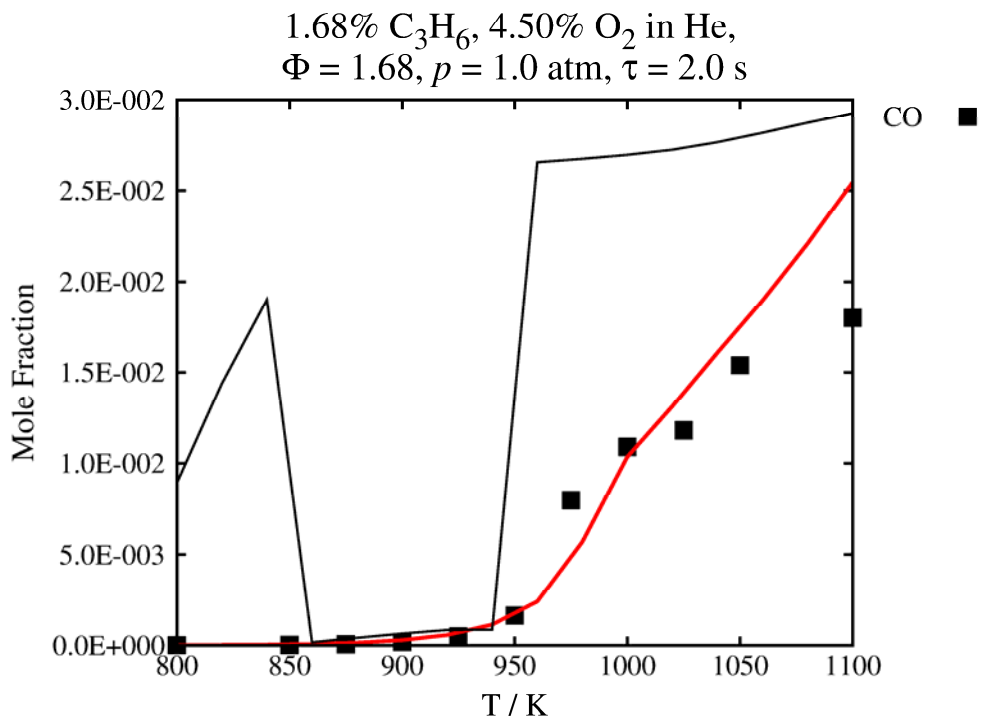
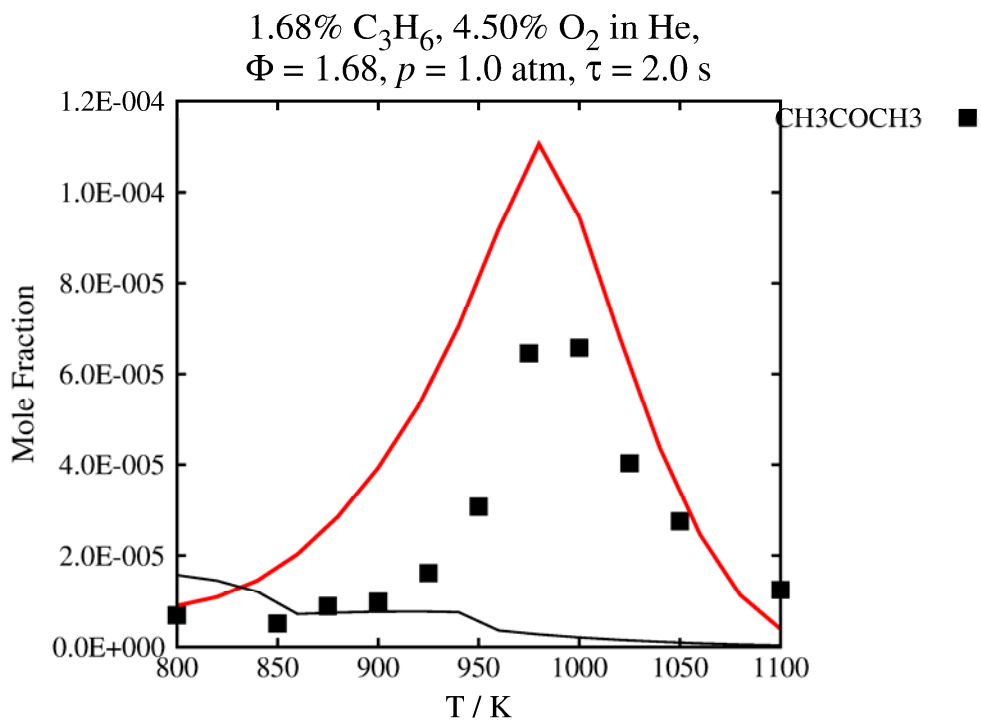
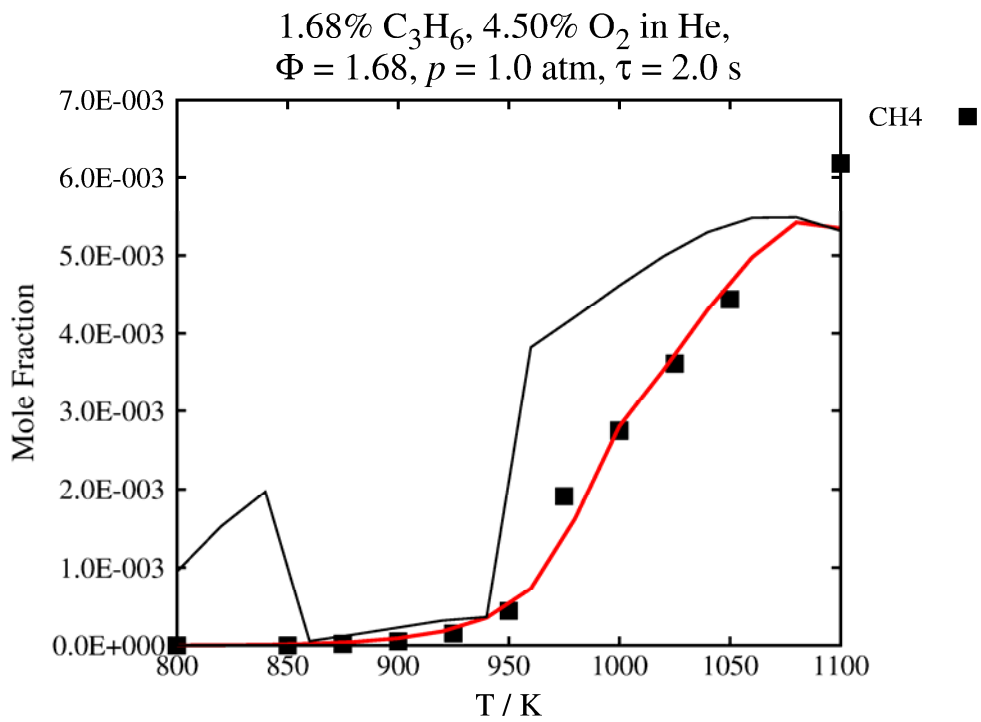
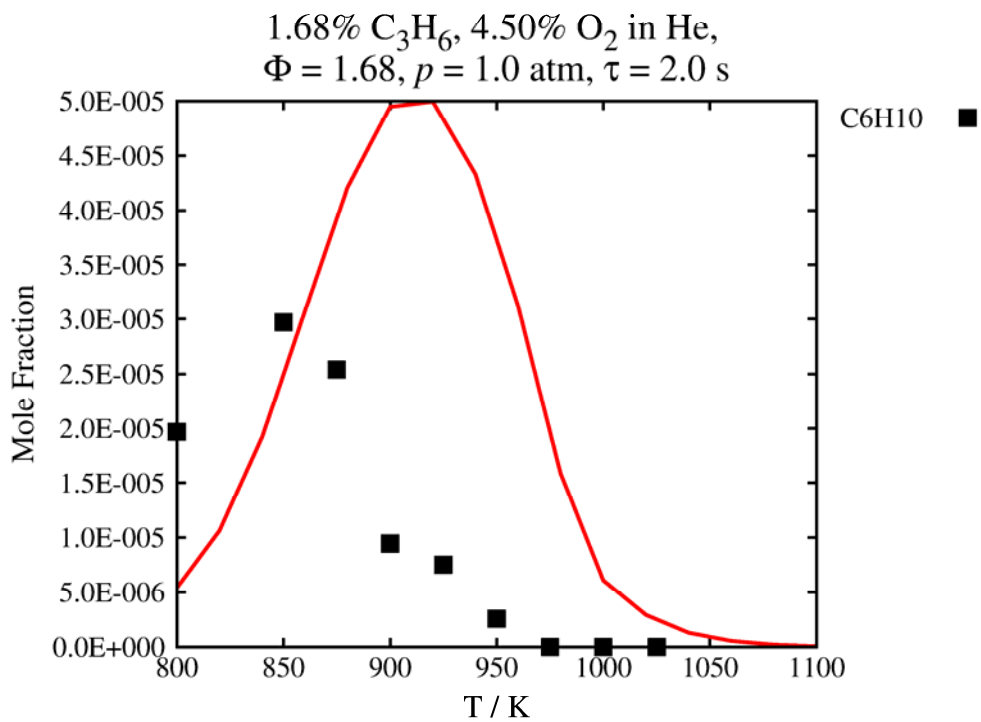
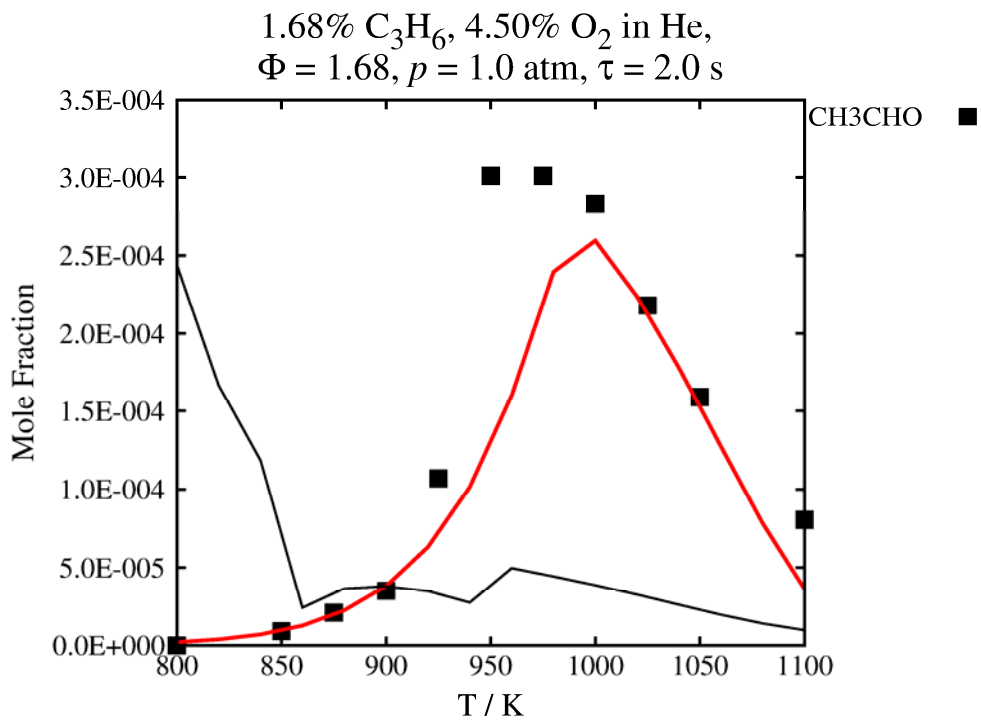


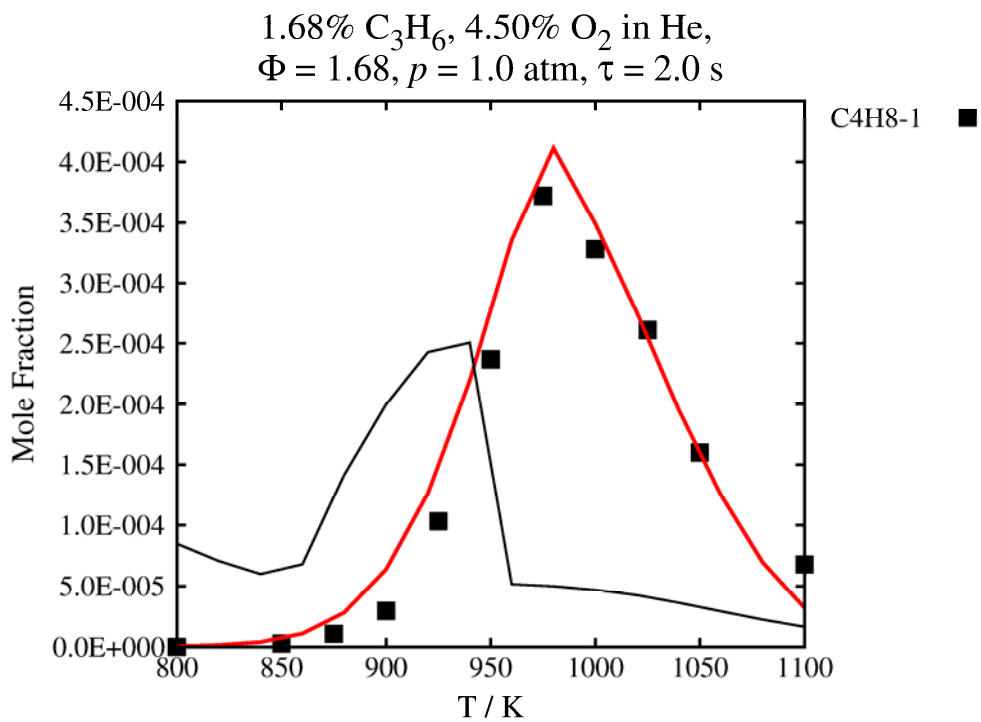
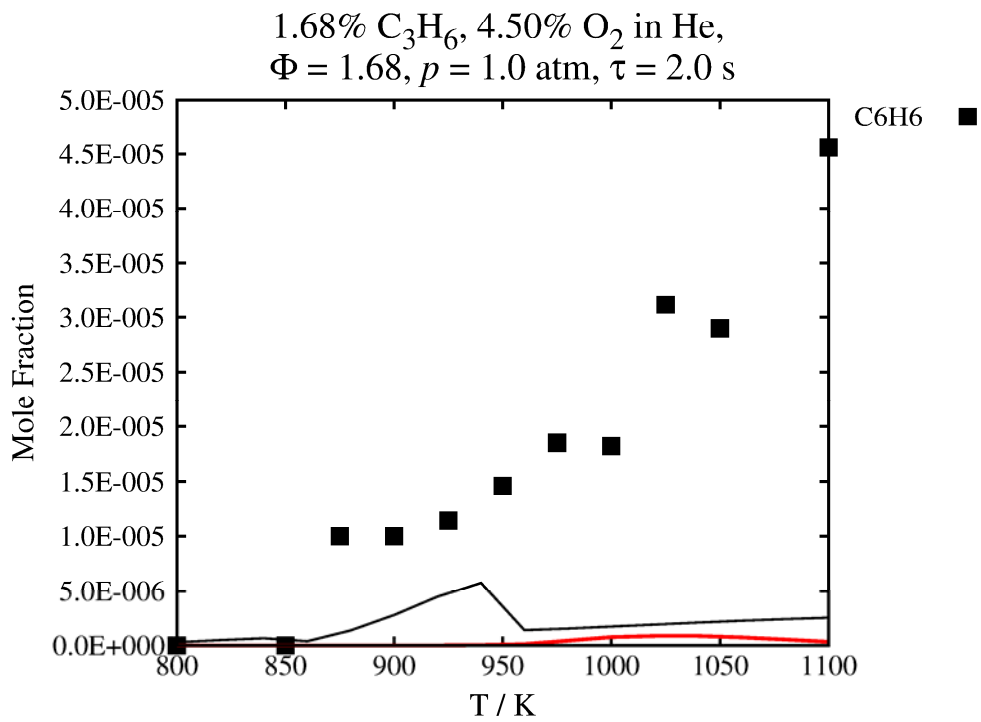
Figure 21 Jet-stirred reactor of propene/O₂/He. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

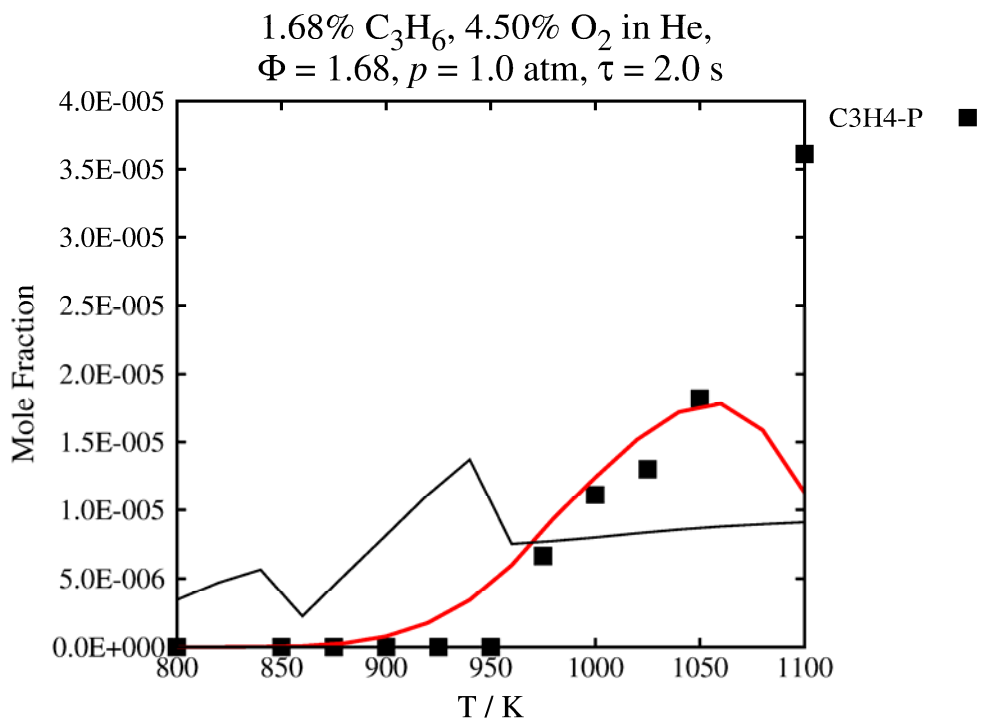
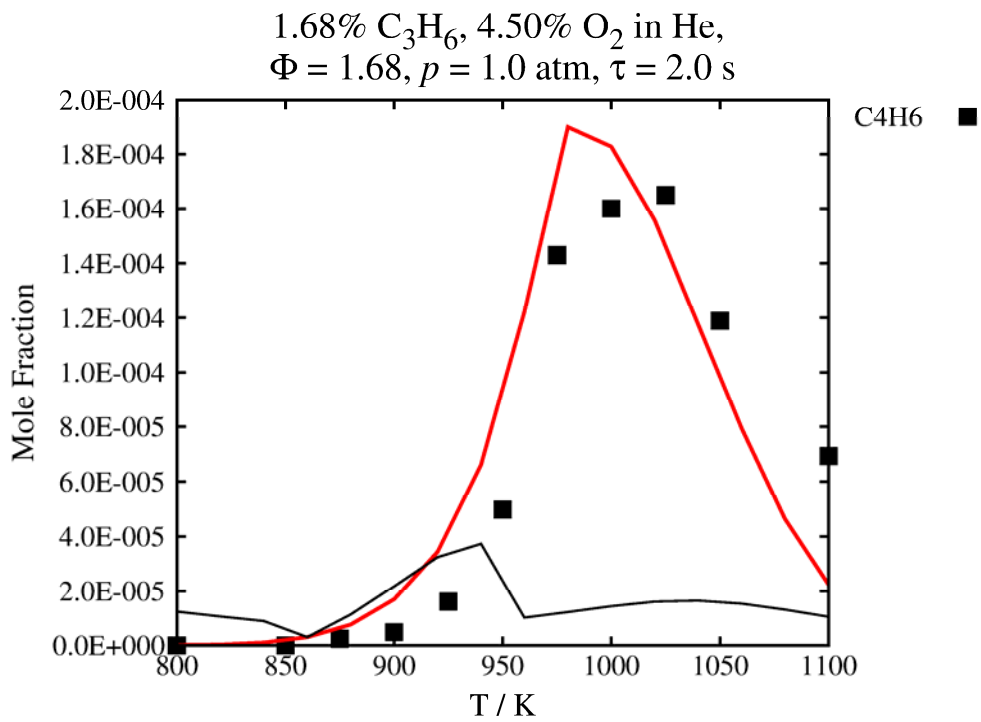


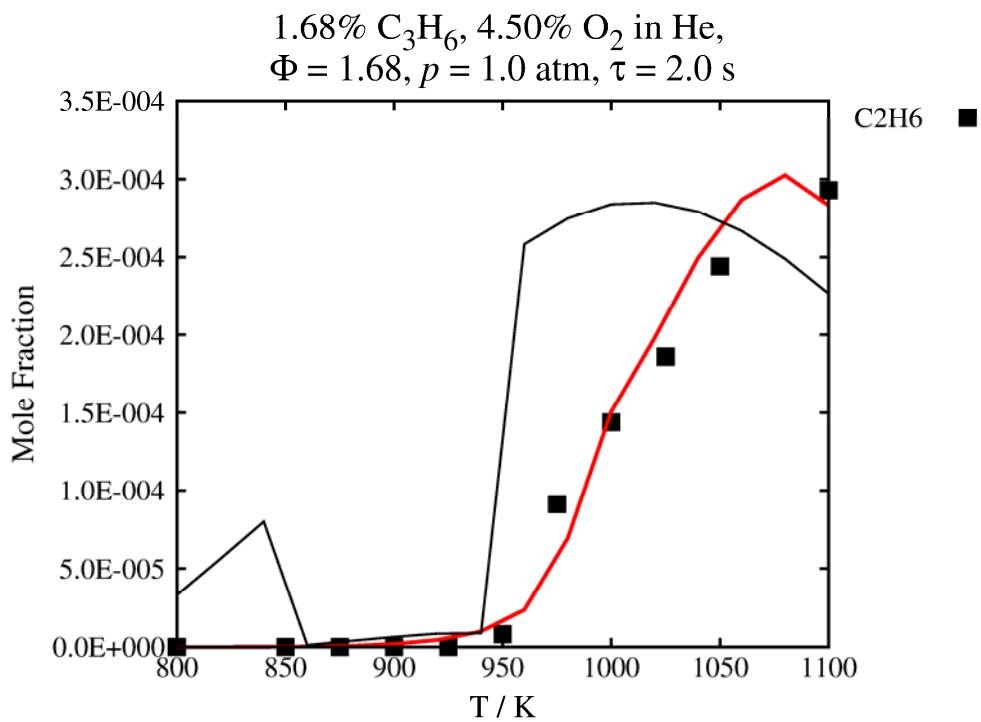
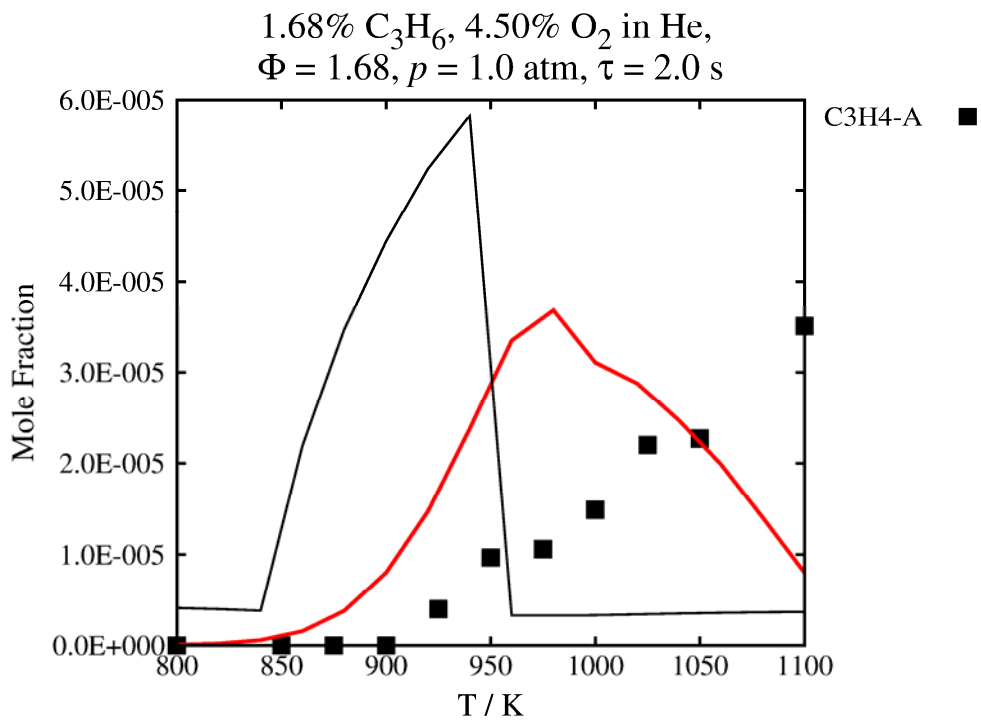


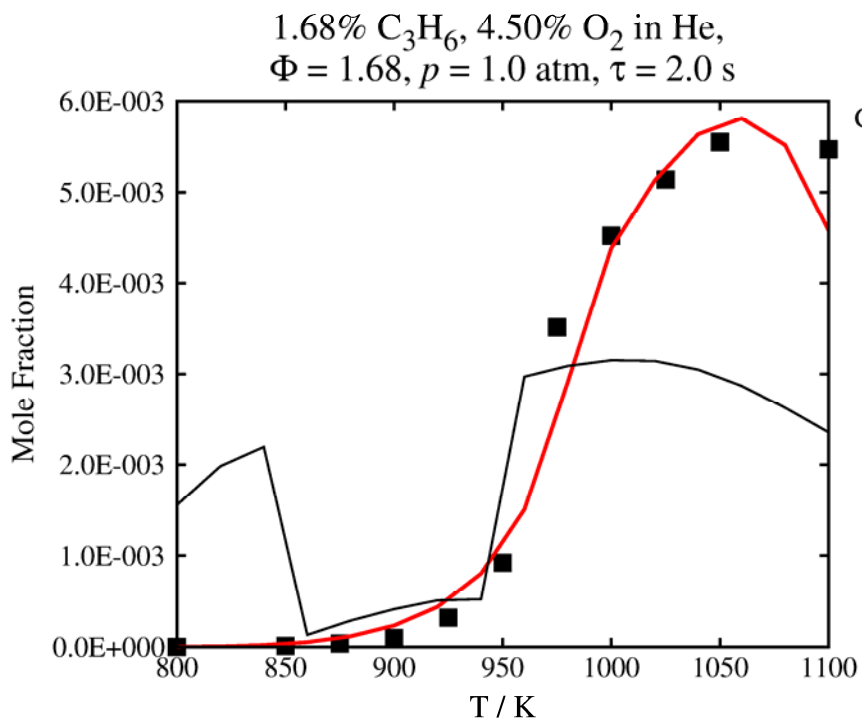
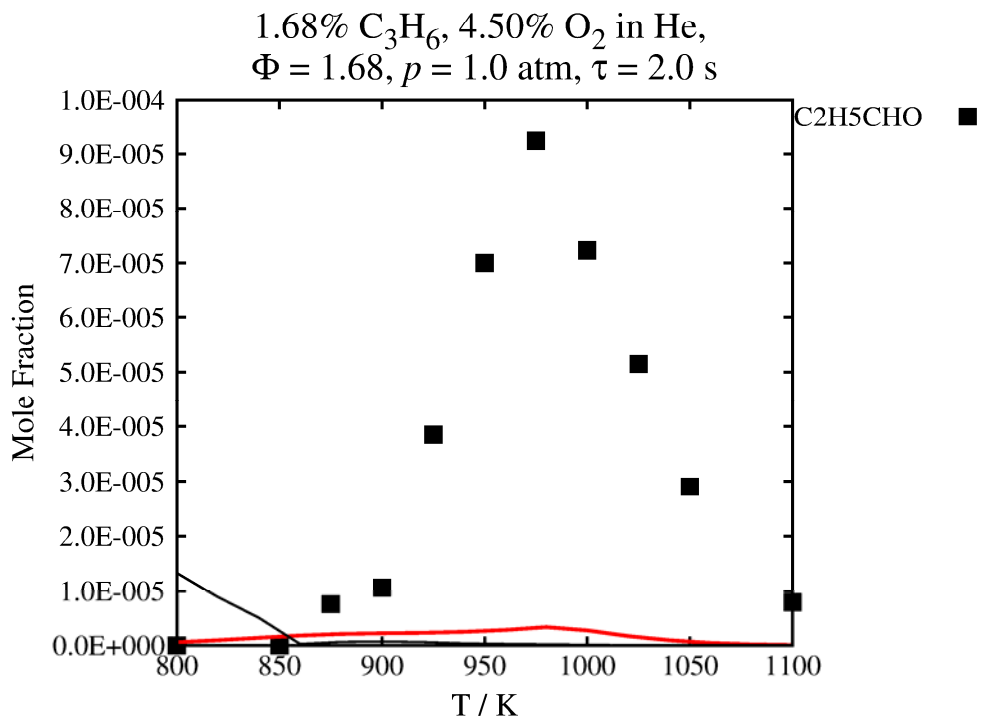












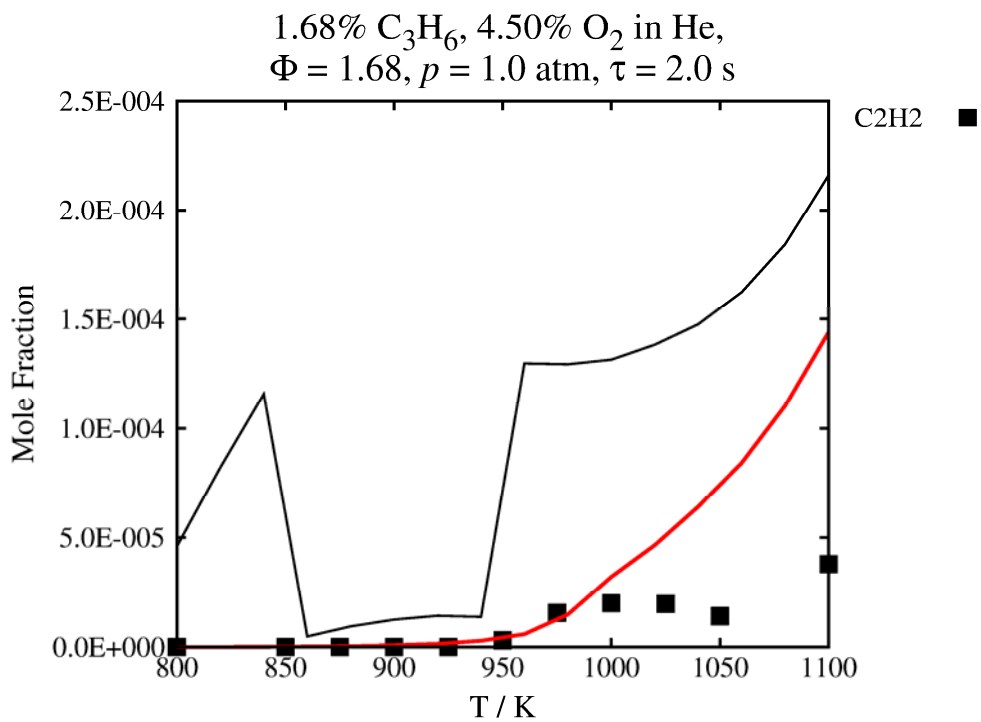
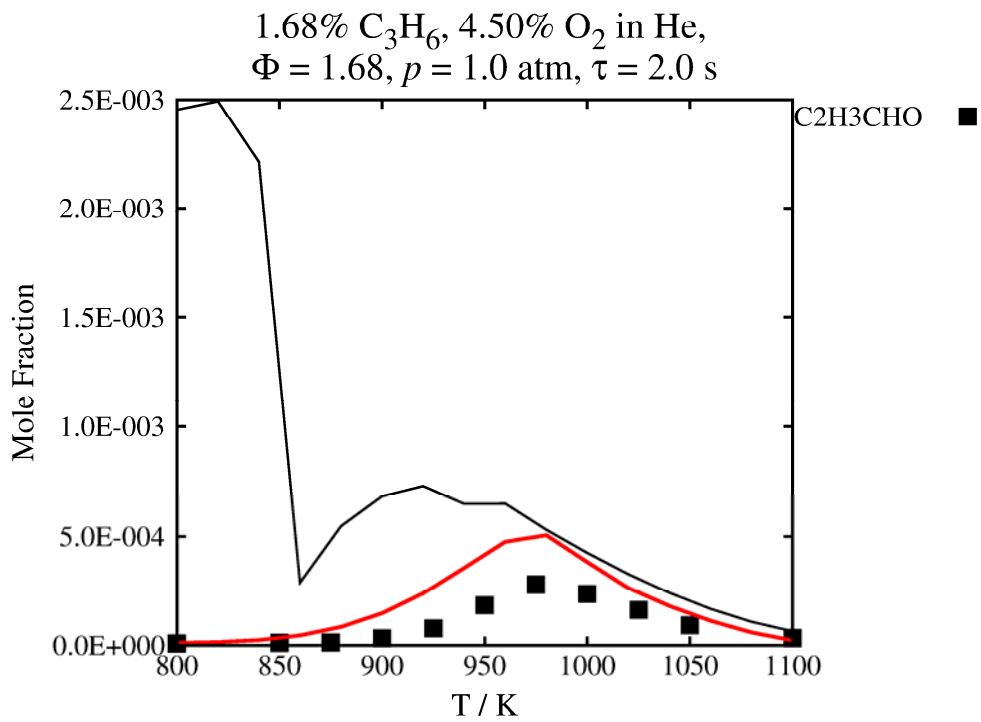
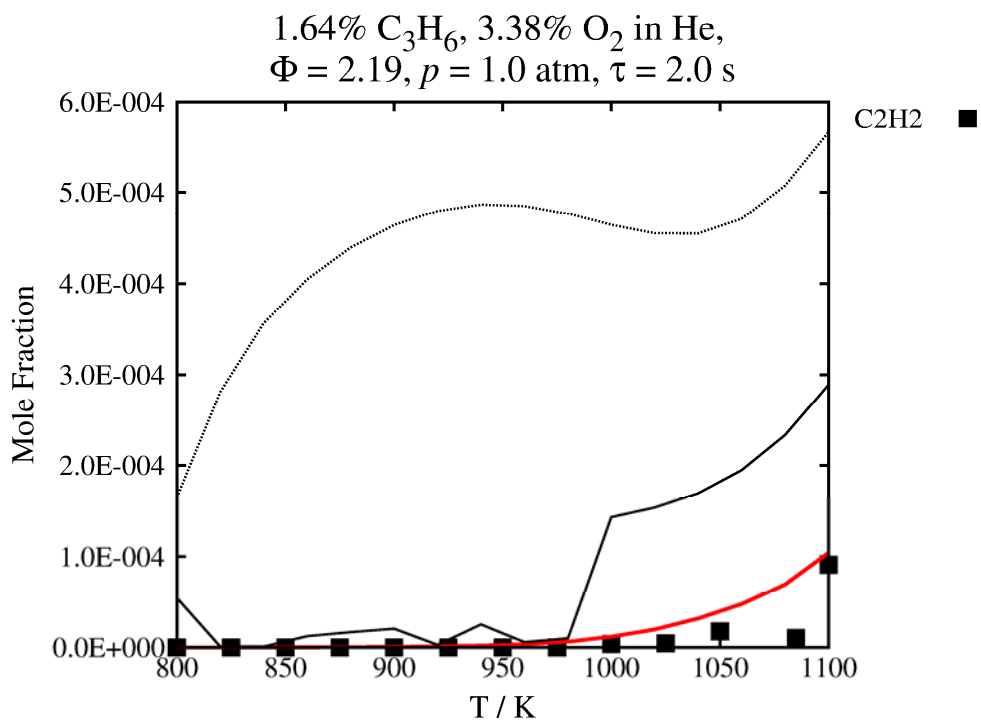
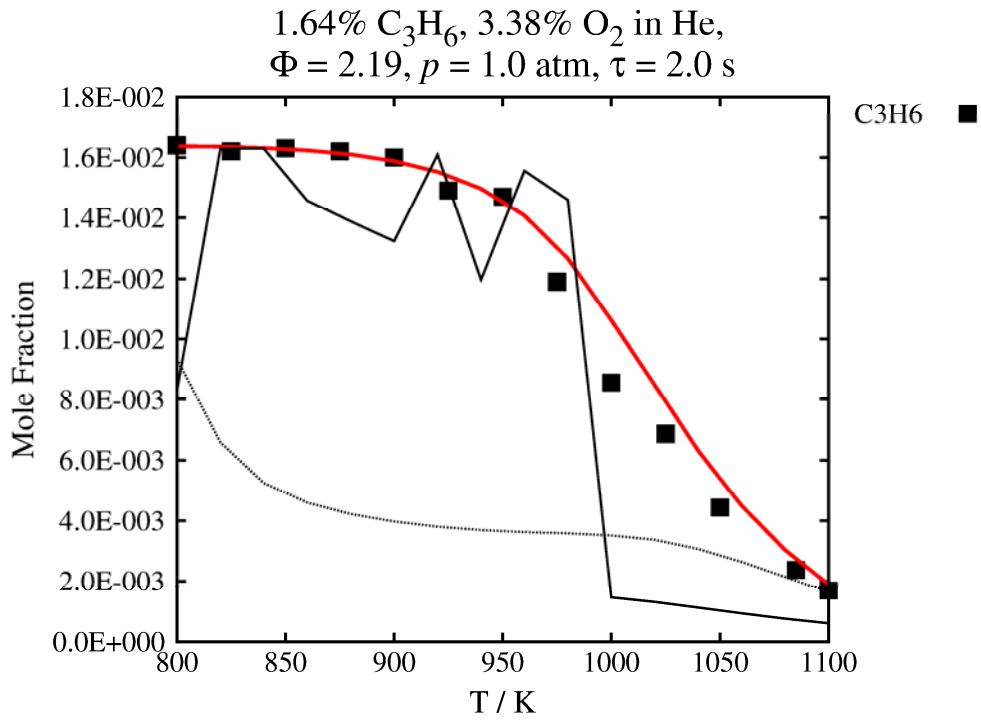
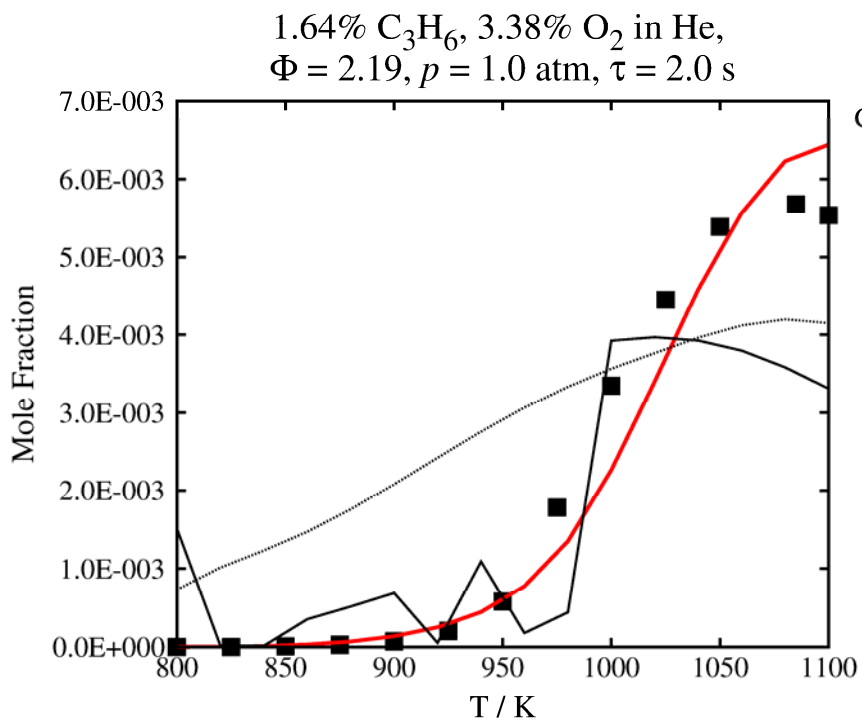
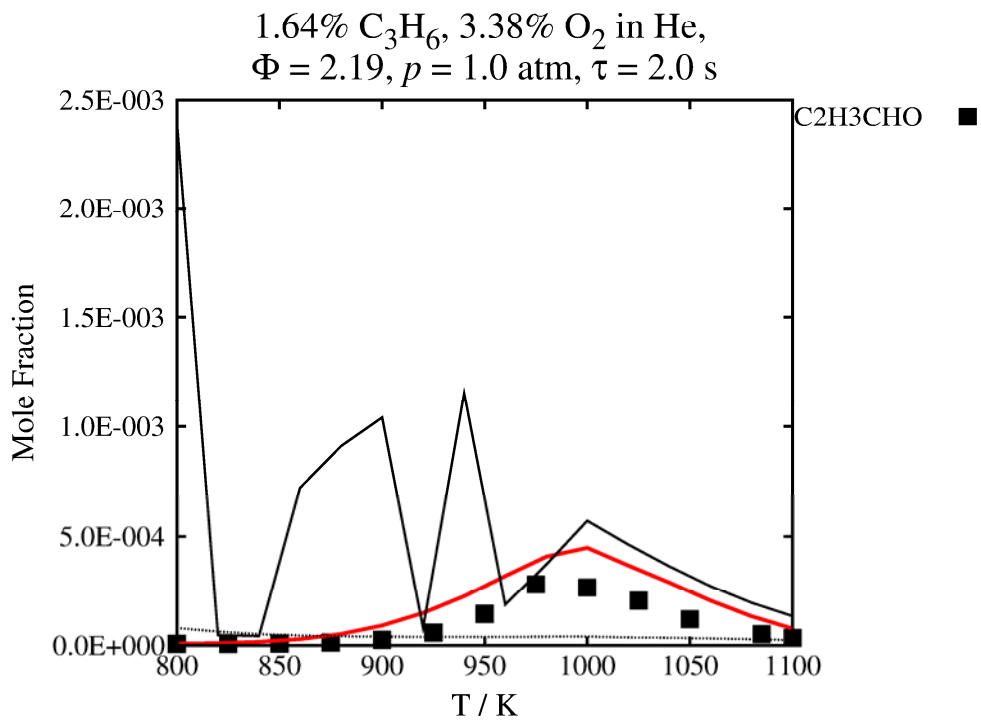
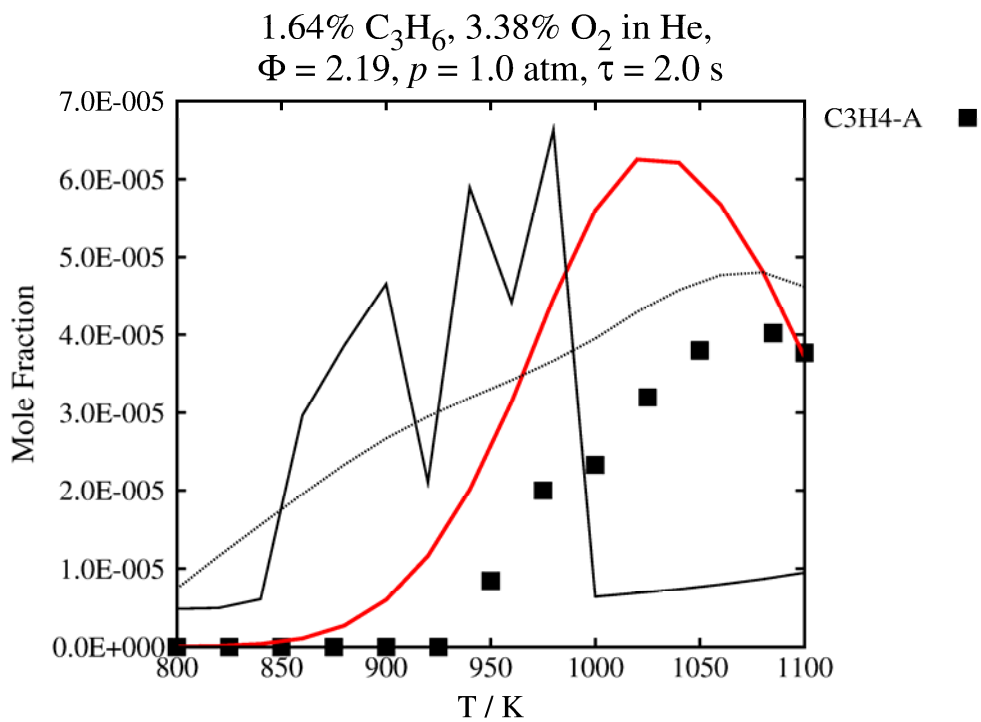
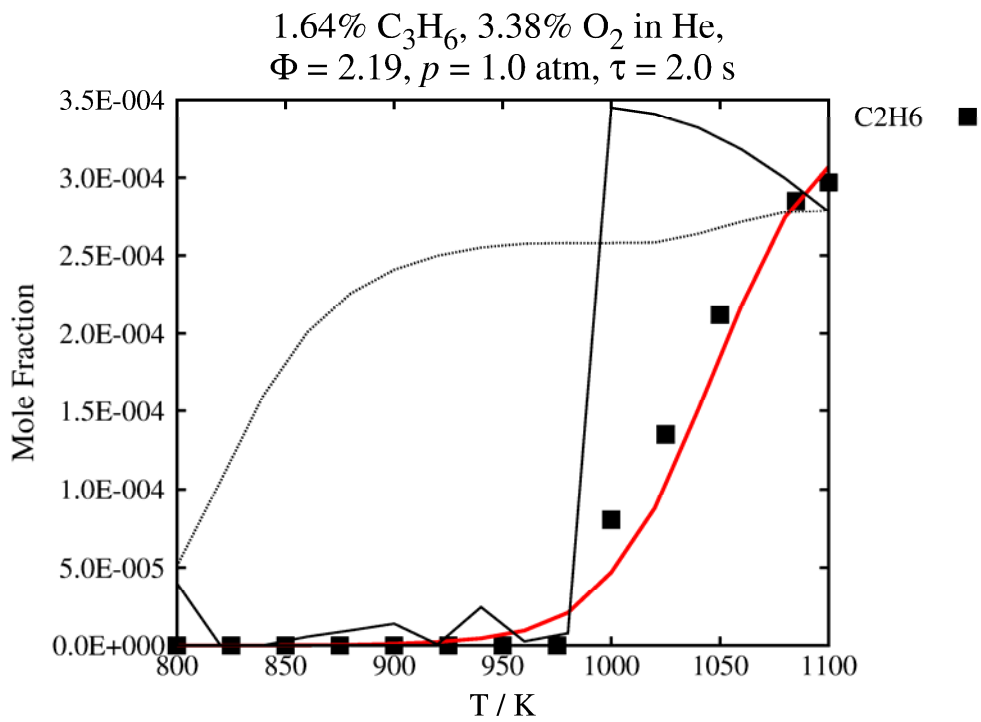
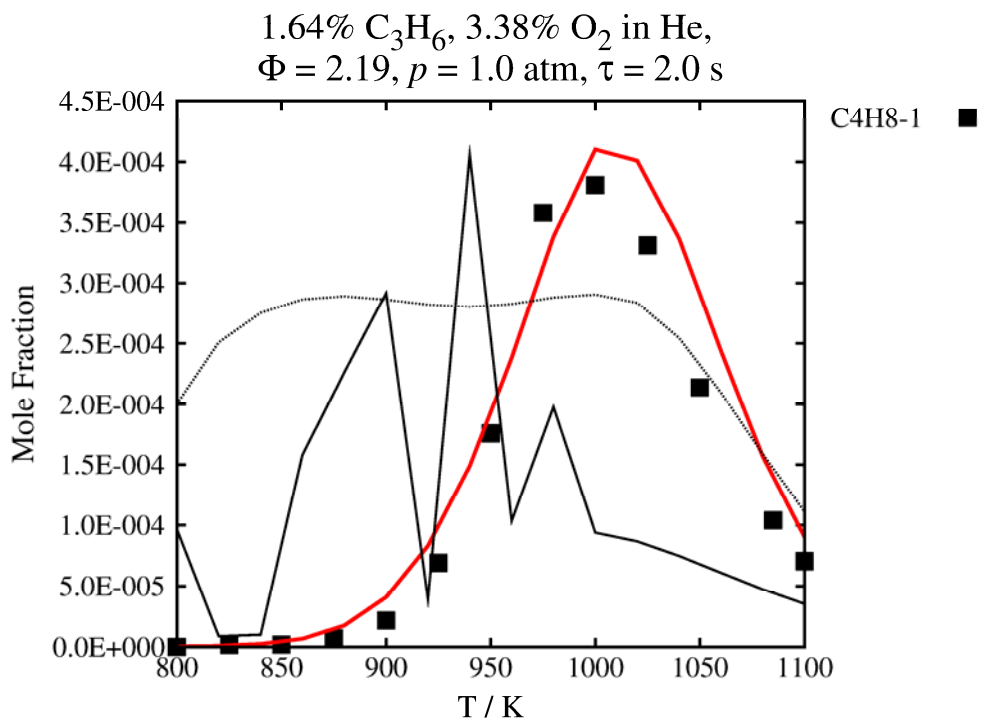
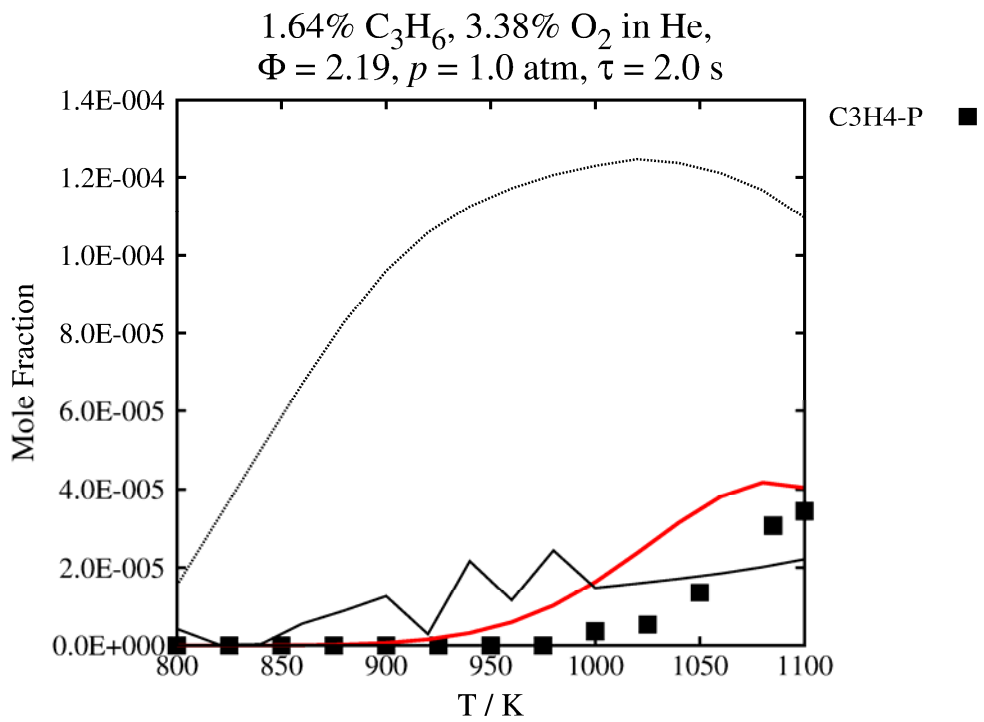


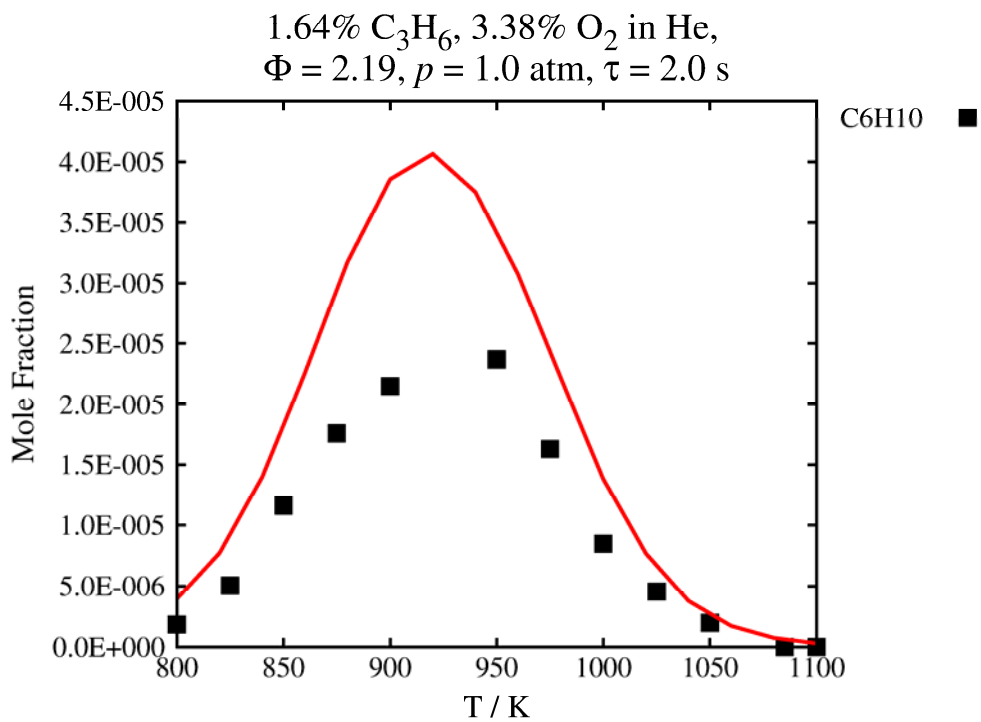
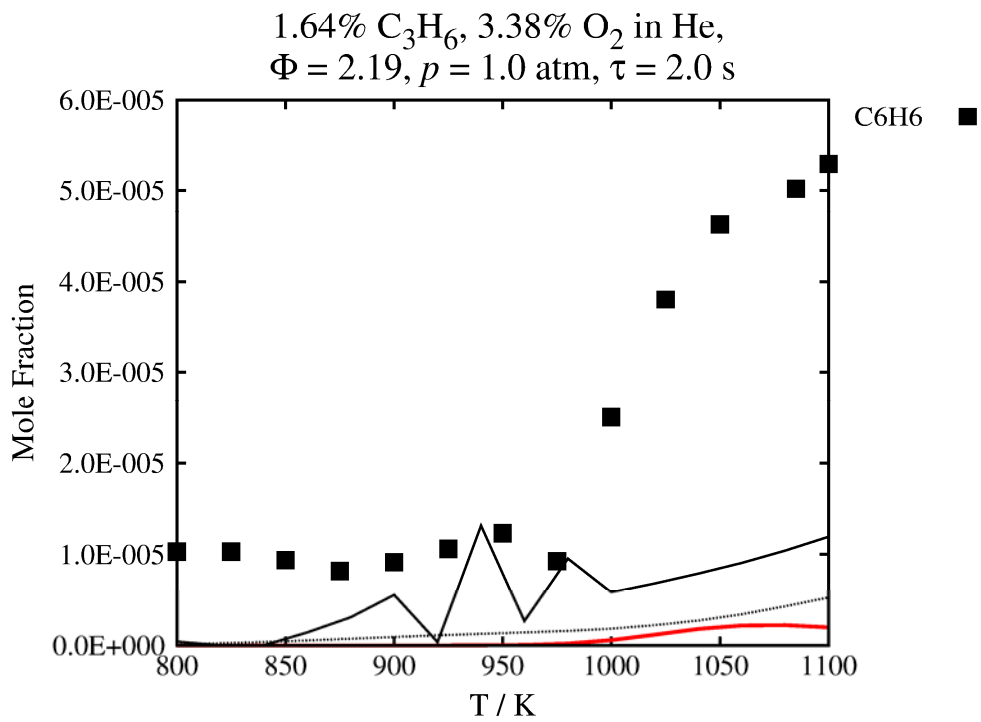
Figure 22 Jet-stirred reactor of propene/O₂/He. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

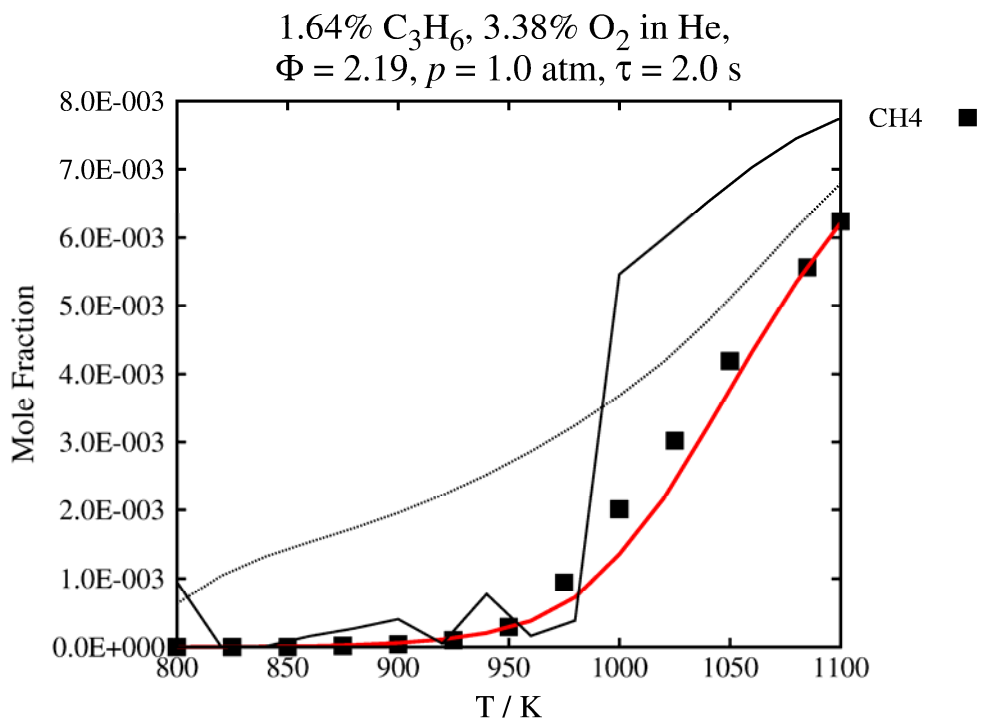
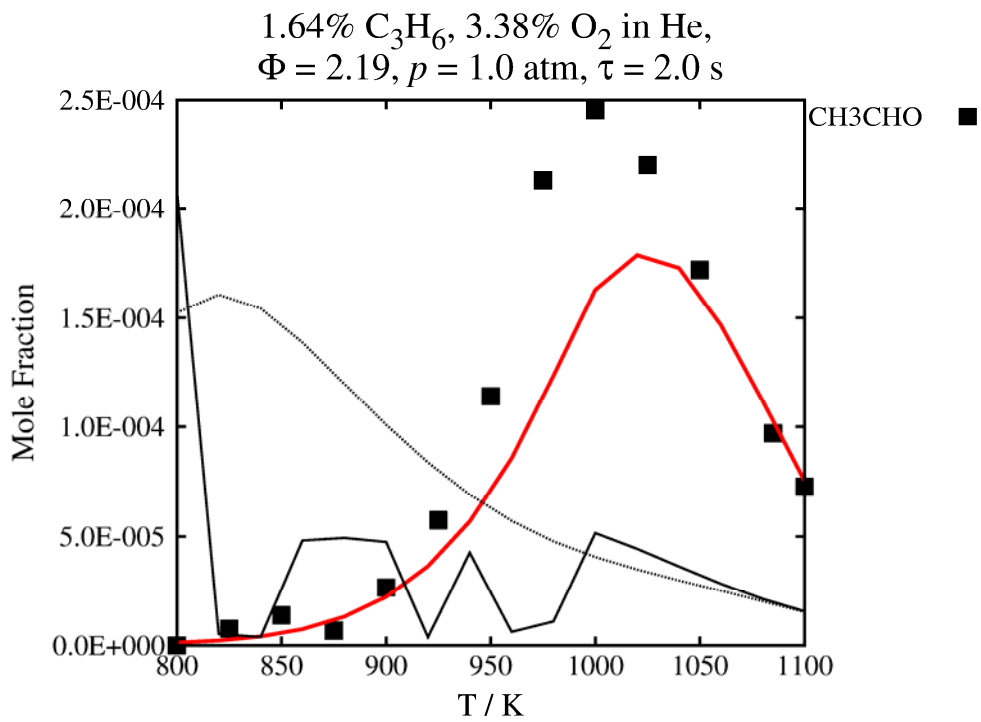












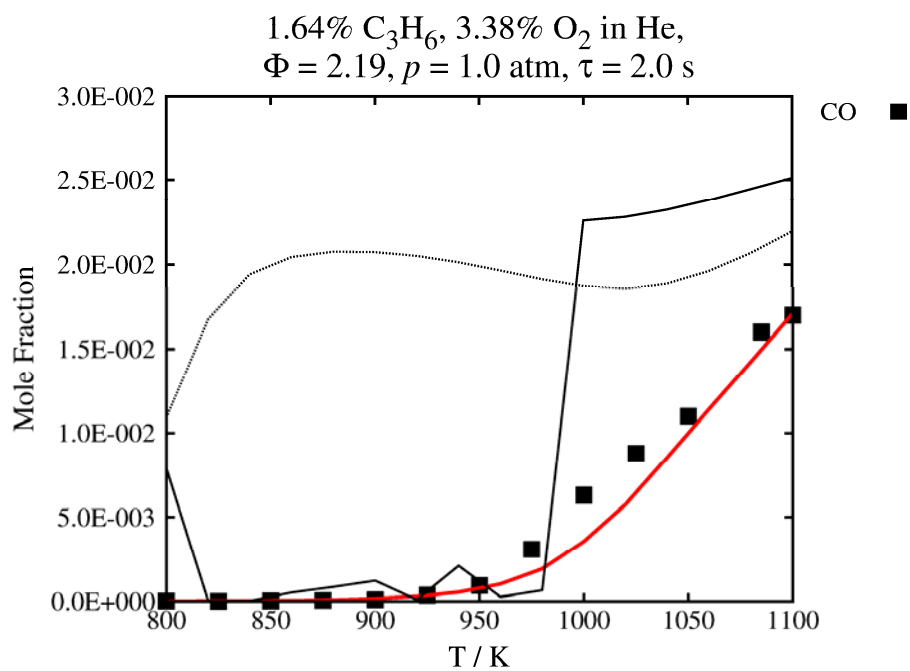
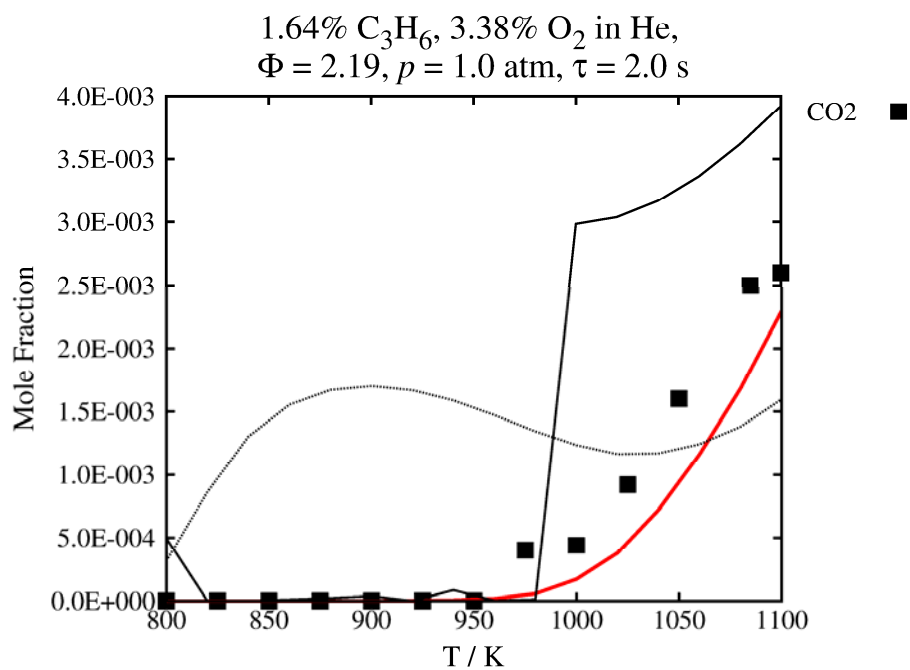
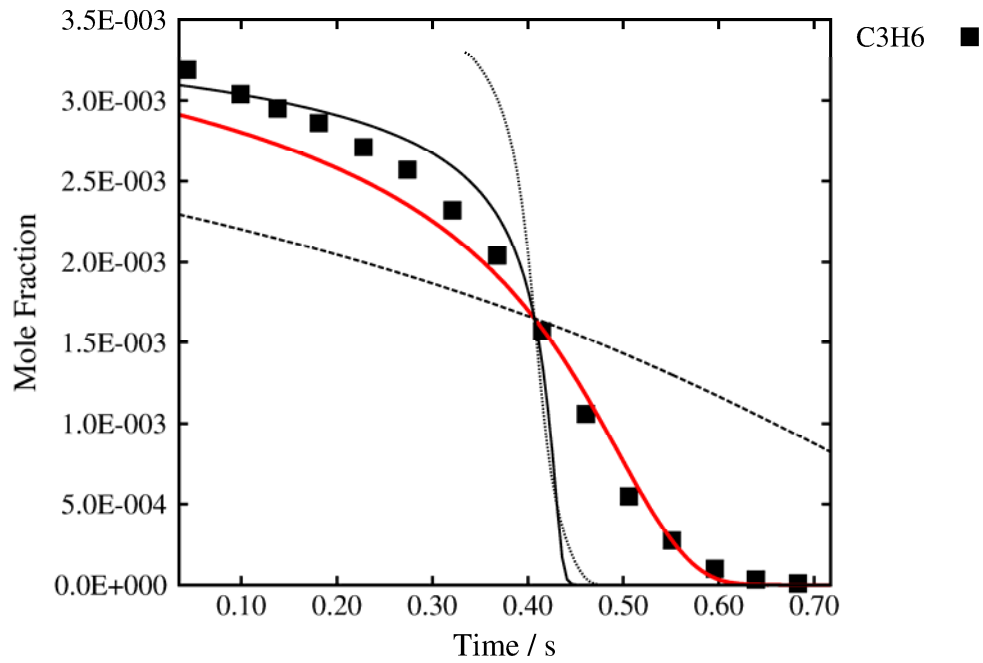


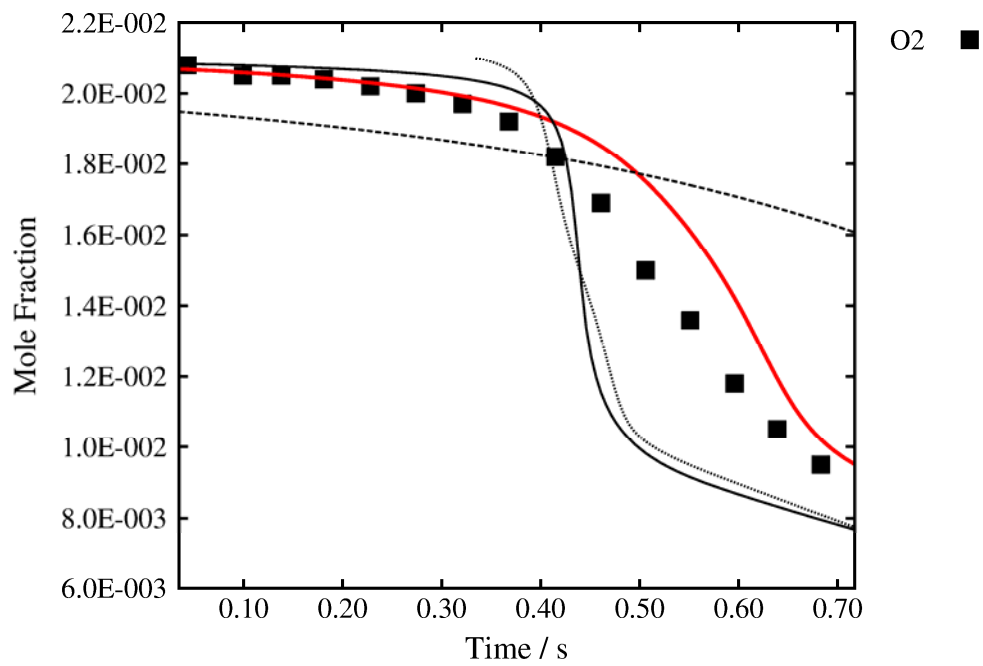
Figure 23 Jet-stirred reactor of propene/O₂/He. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

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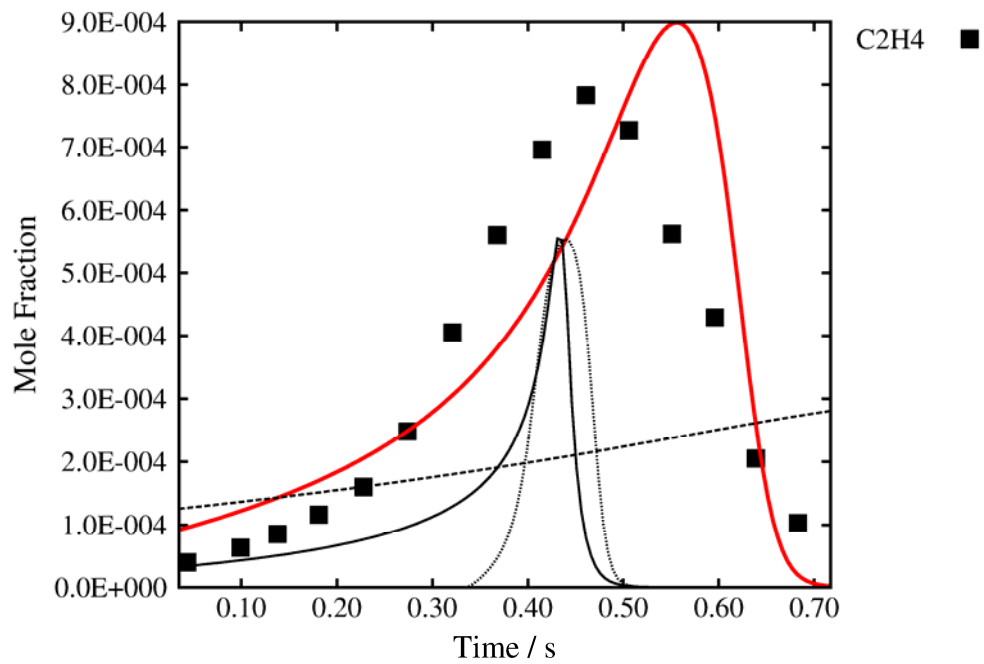
0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



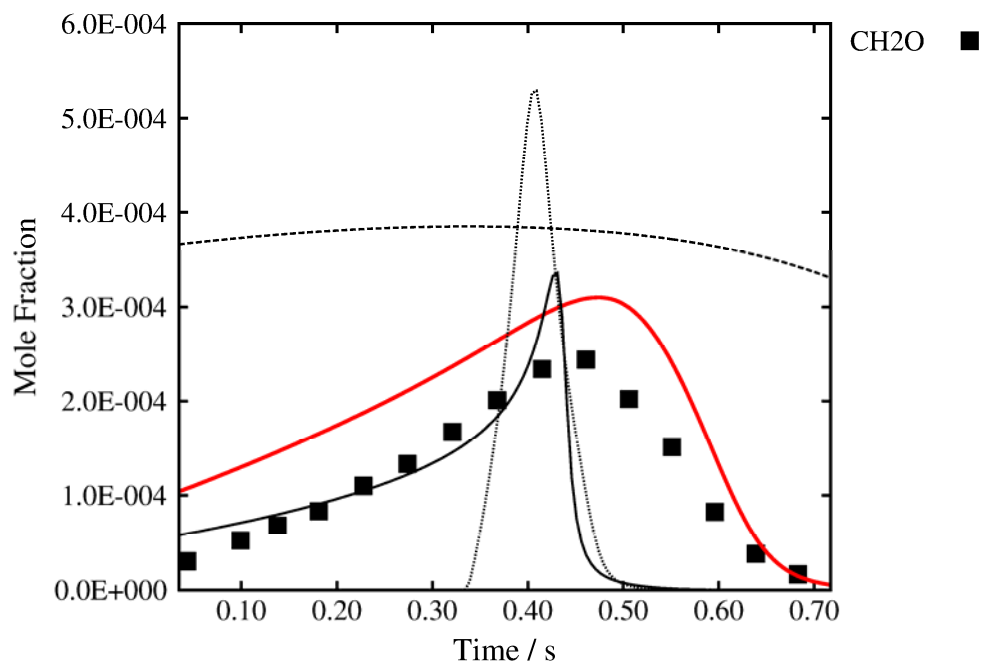
0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



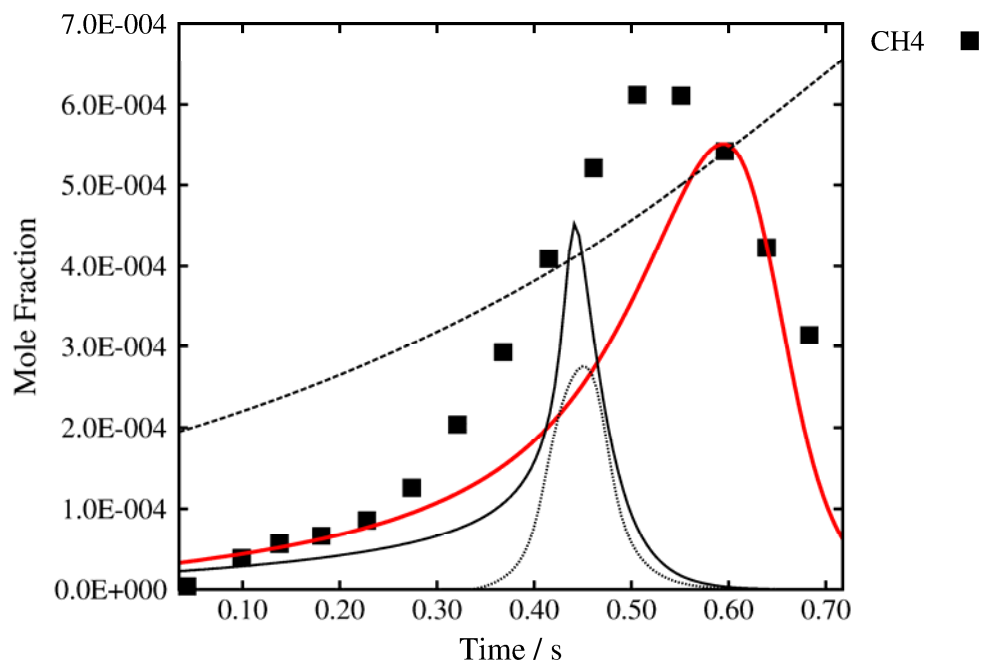
0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



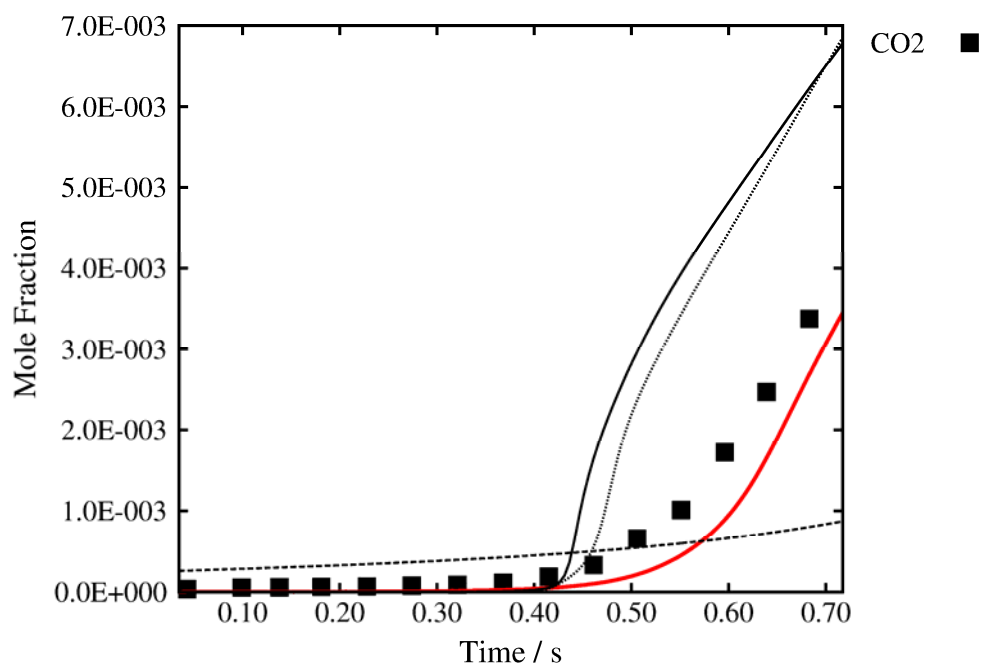
0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



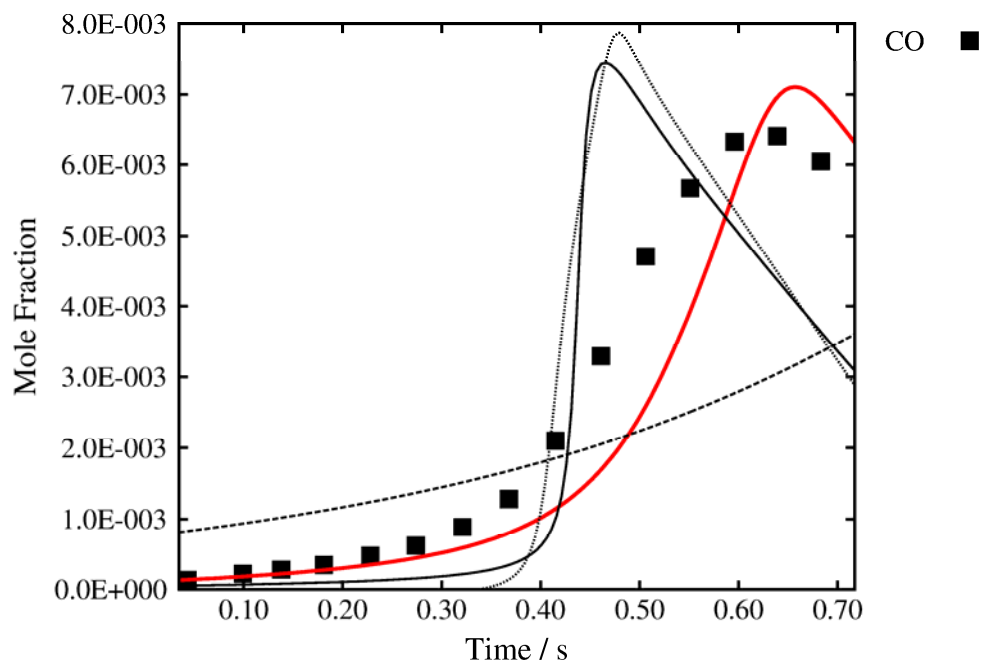
0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K



0.33% C₃H₆ 2.10% O₂ in N₂, $\Phi = 0.71$, $p = 6.0$ atm, $T = 968$ K

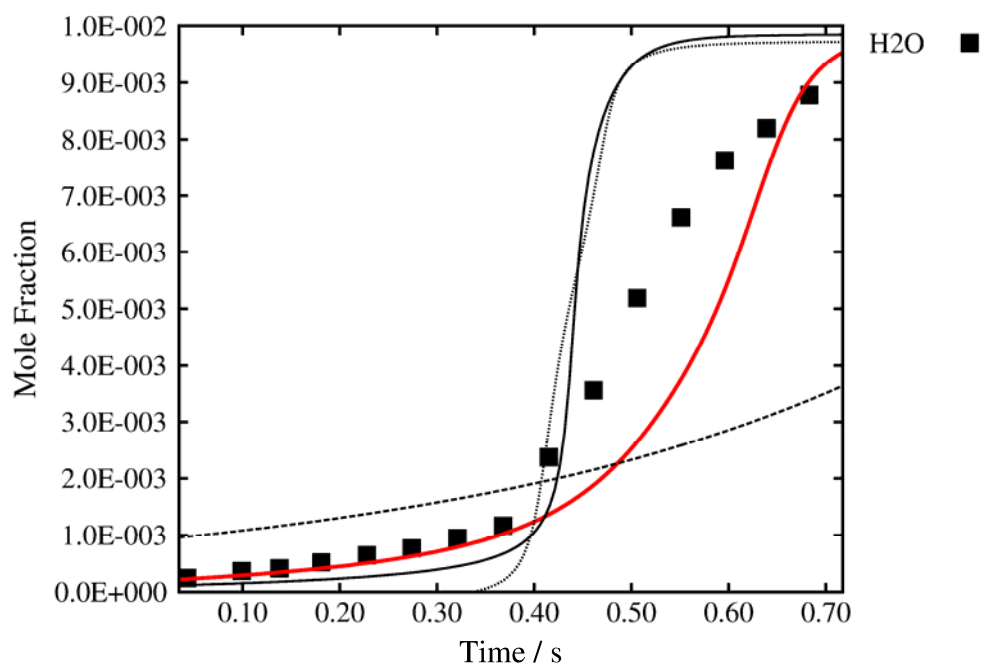
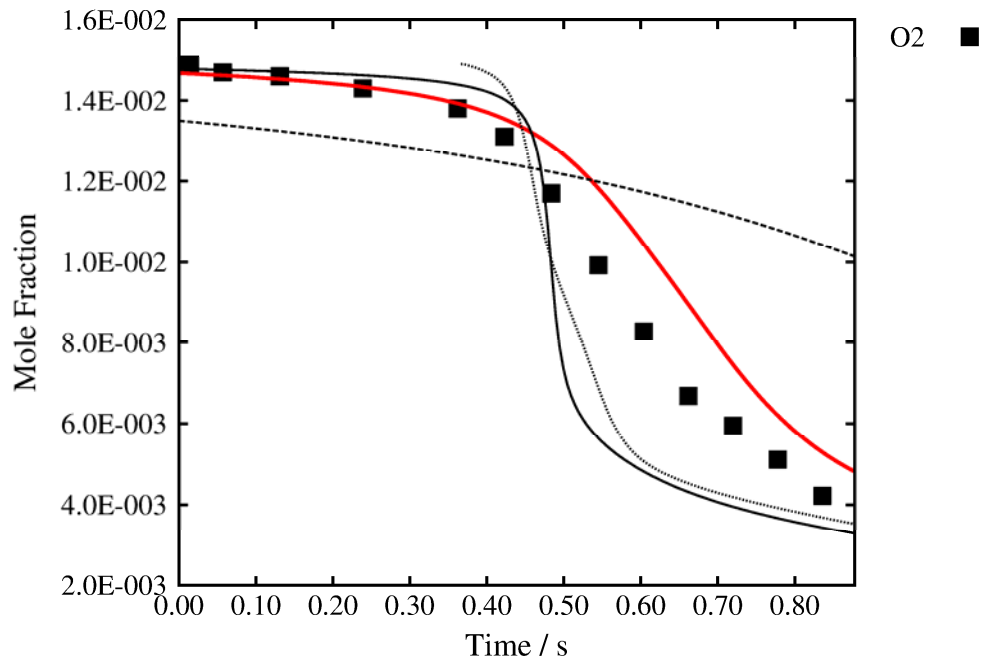
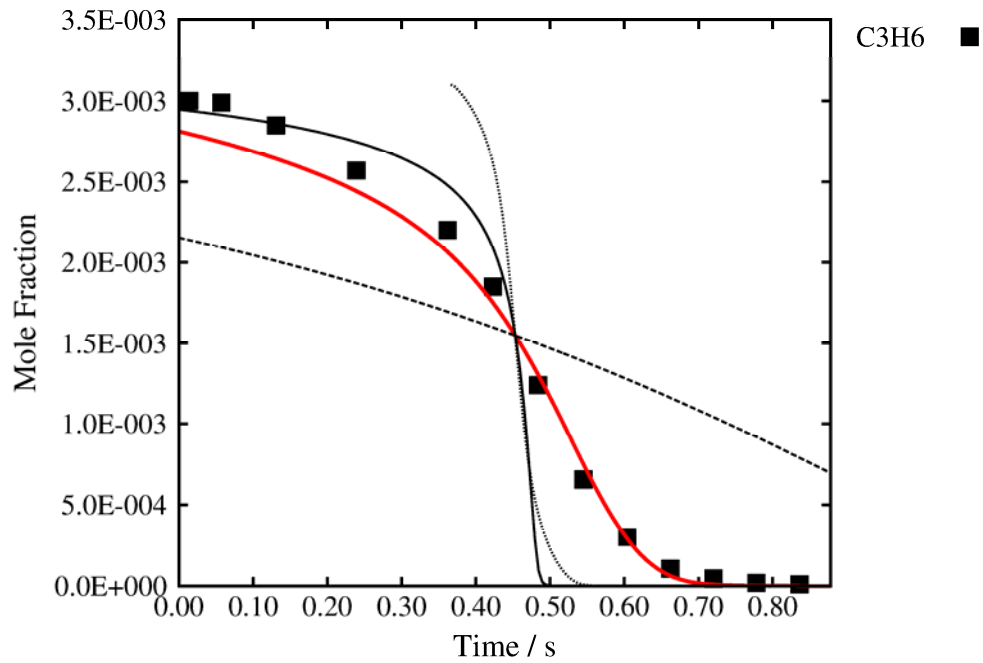


Figure 24 Flow reactor of propene/O₂/N₂. Symbols are experimental data (this study) lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

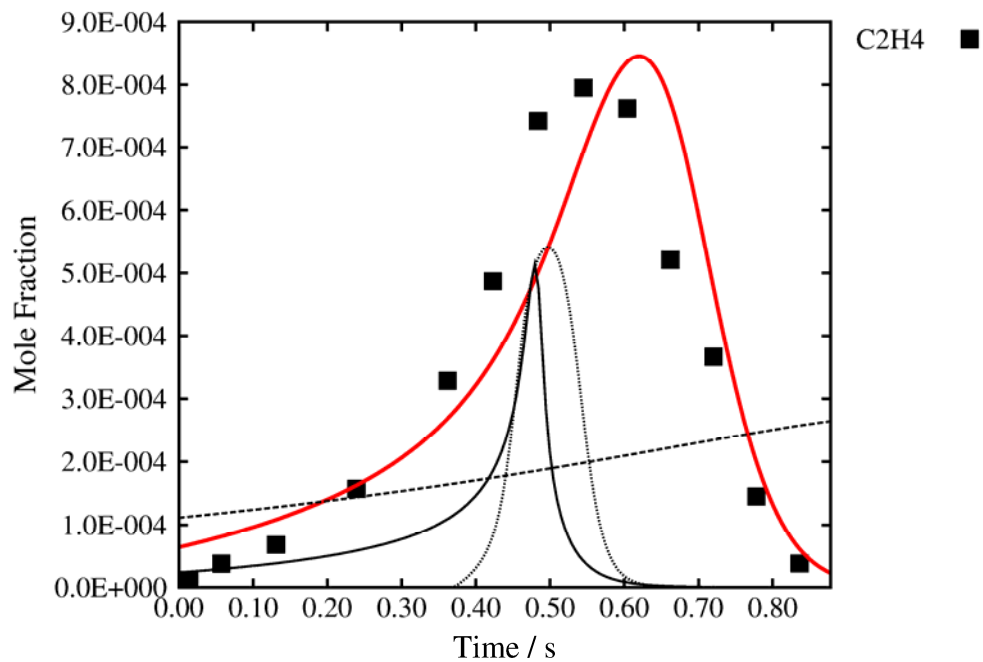
0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



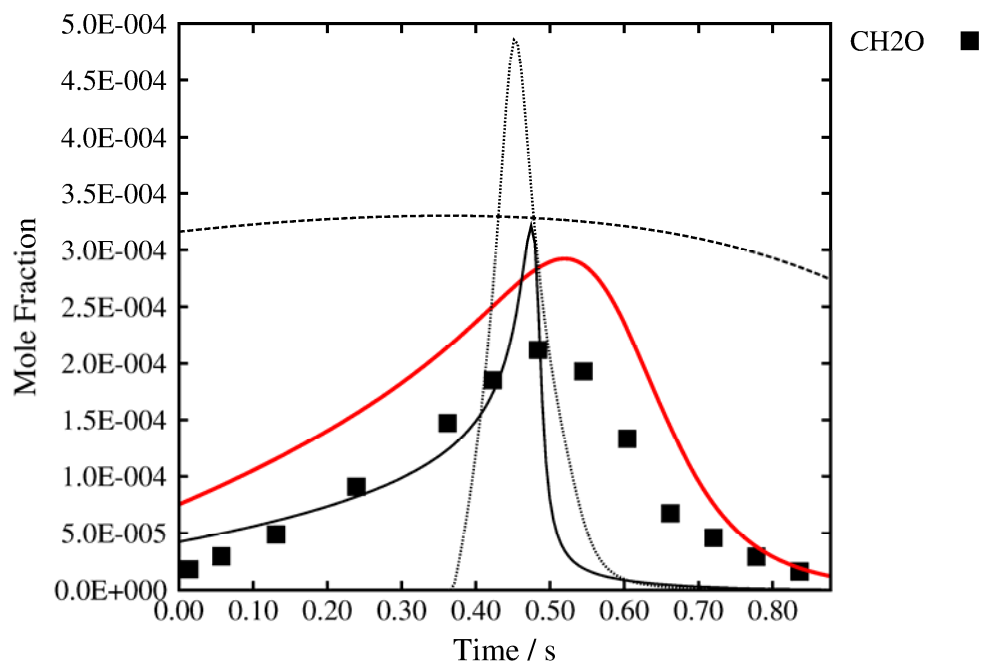
0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



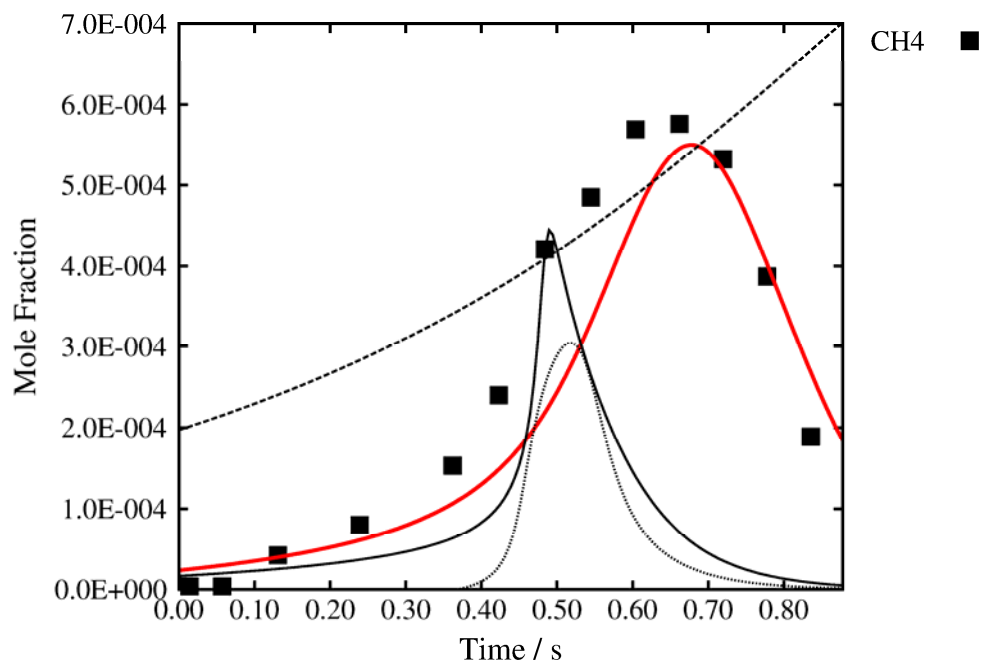
0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



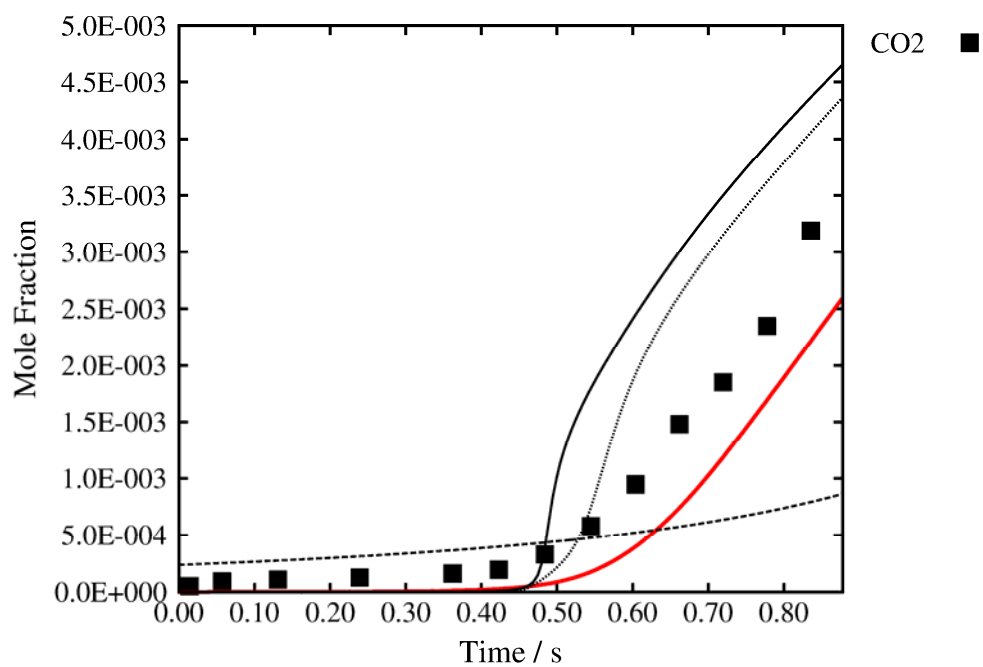
0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



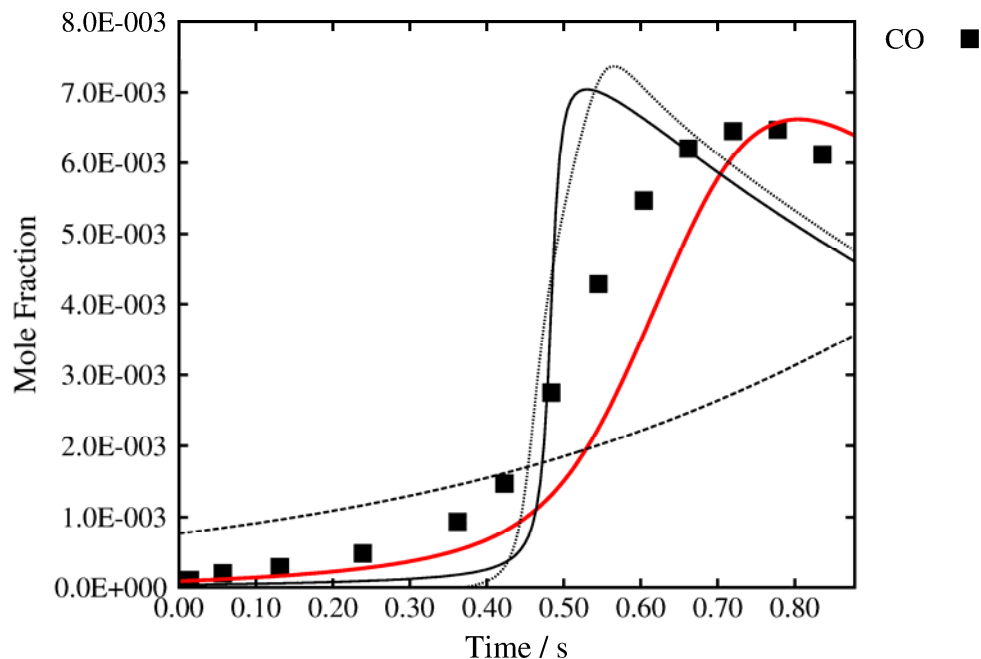
0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K



0.31% C₃H₆ 1.49% O₂ in N₂, $\Phi = 0.94$, $p = 8.0$ atm, $T = 955$ K

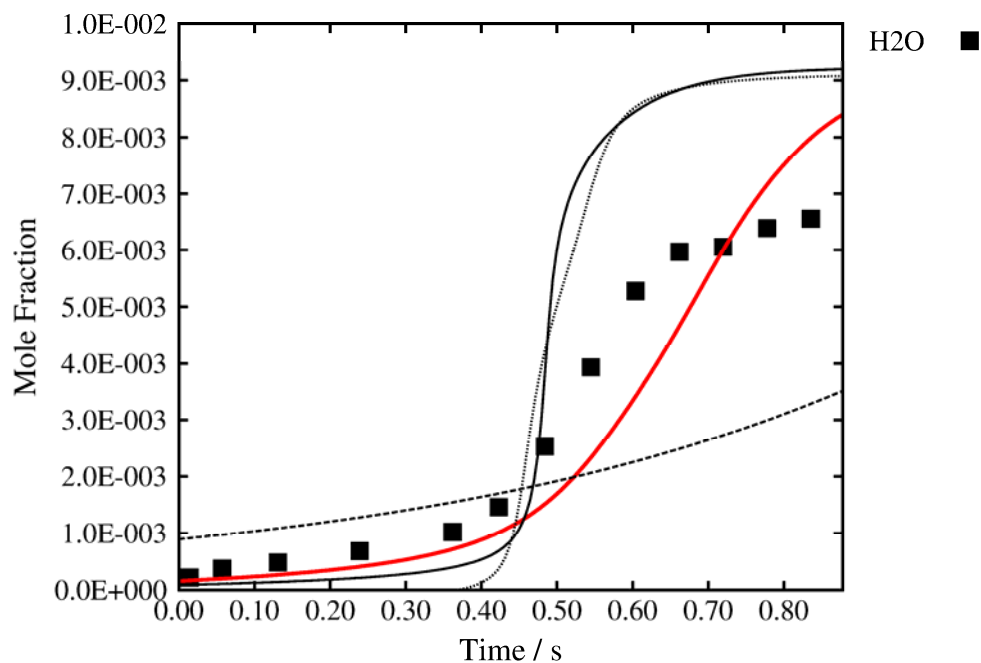
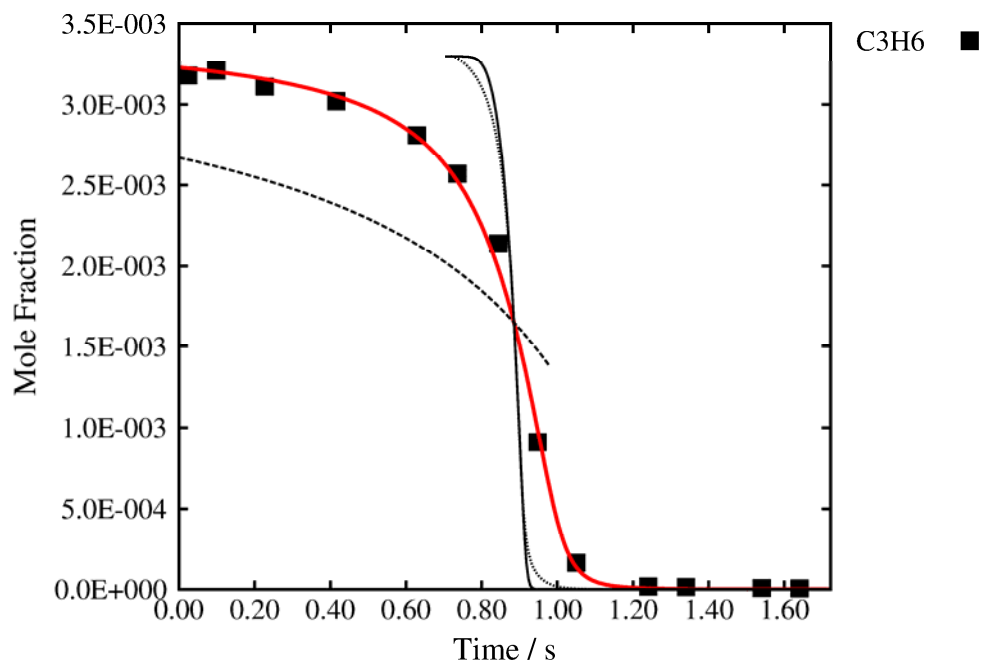
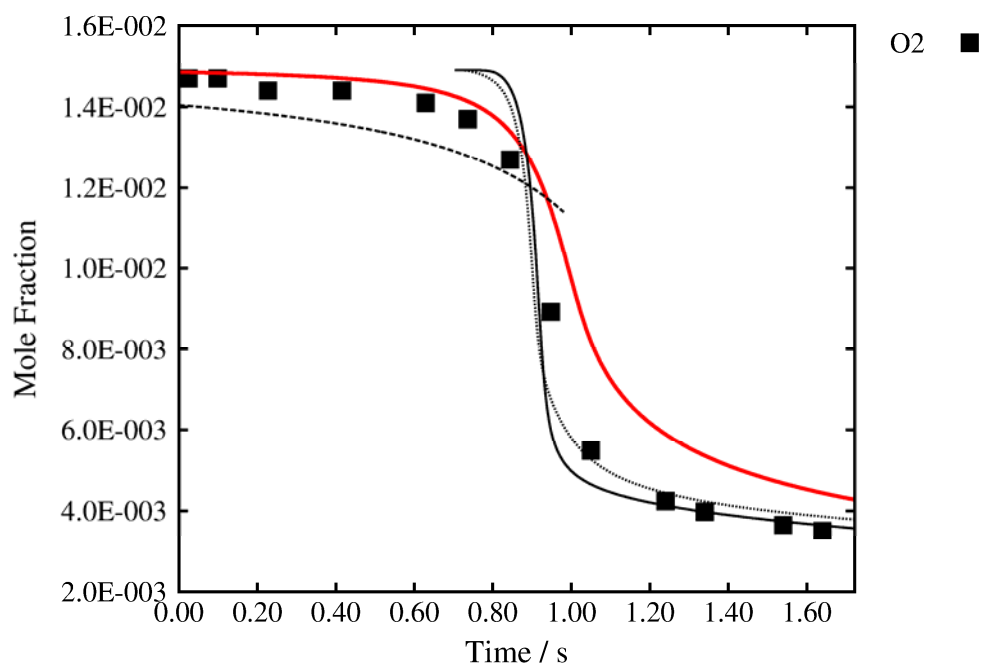


Figure 25 Flow reactor of propene/O₂/N₂. Symbols are experimental data (this study) lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

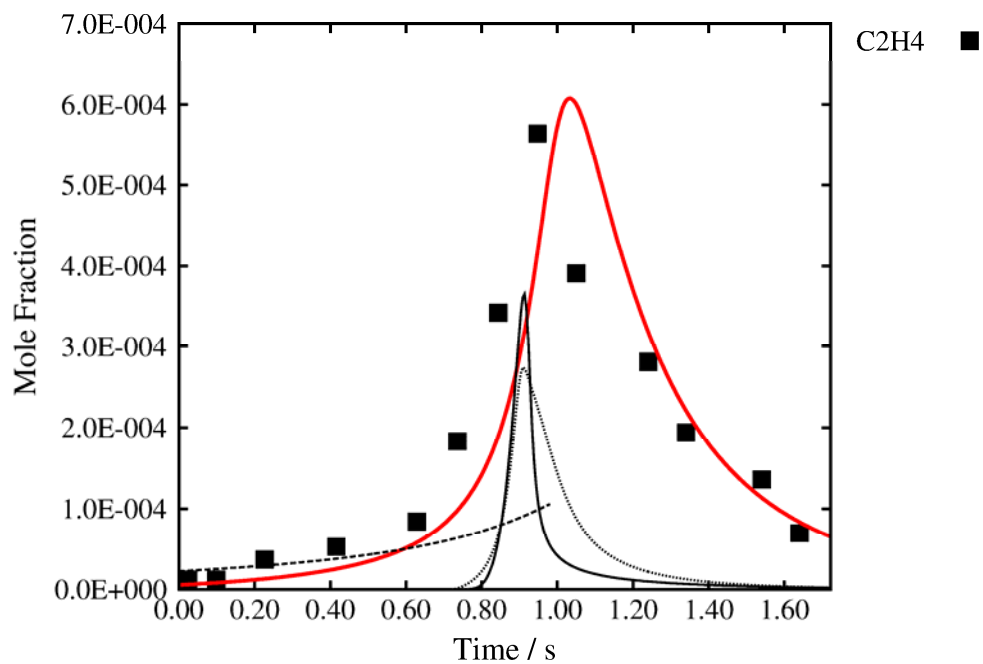
0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



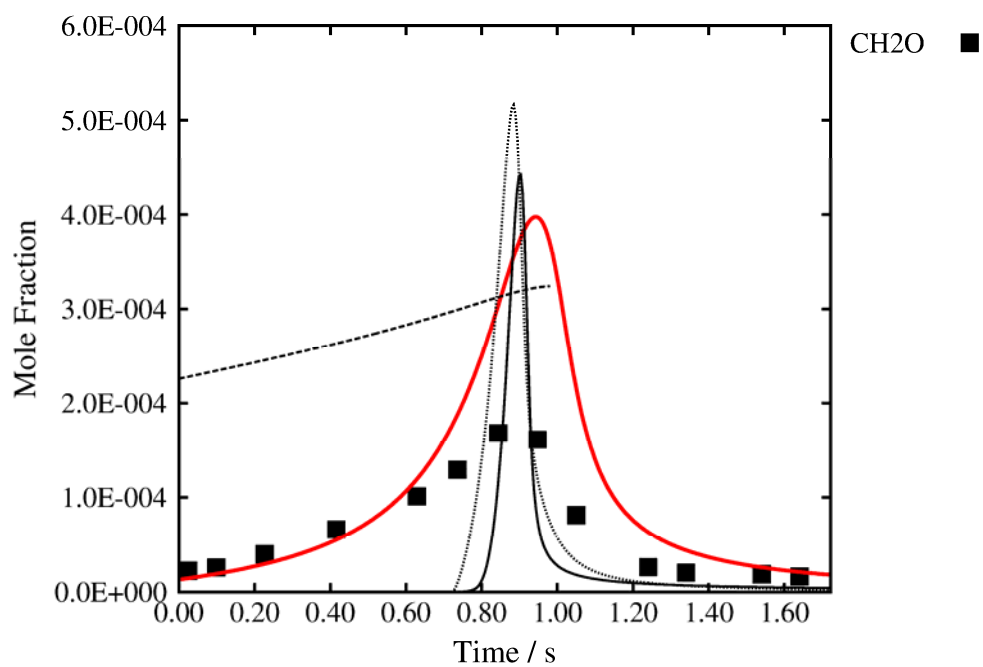
0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



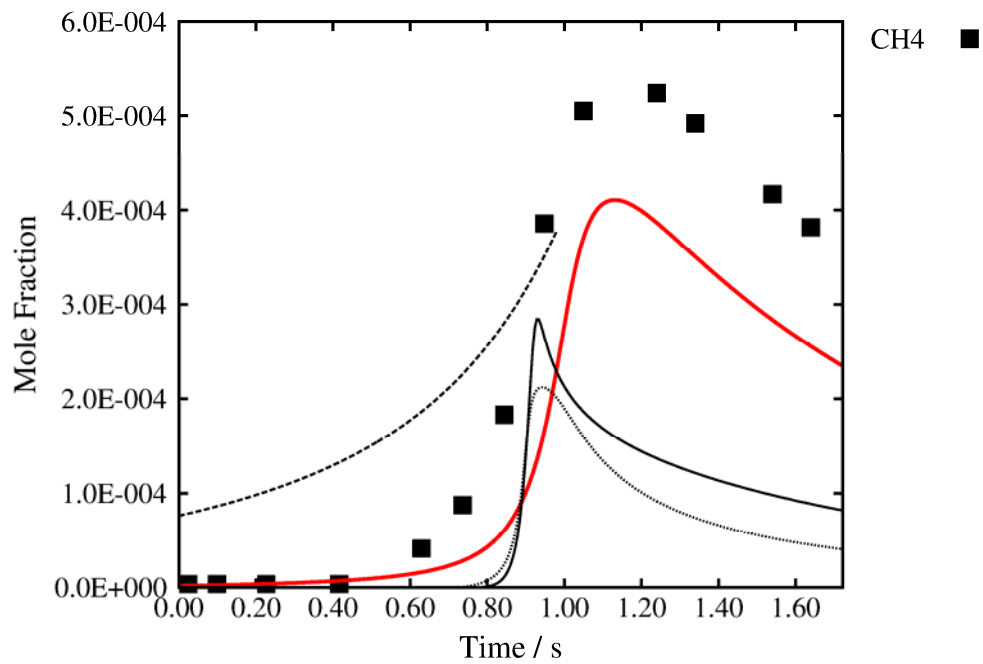
0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



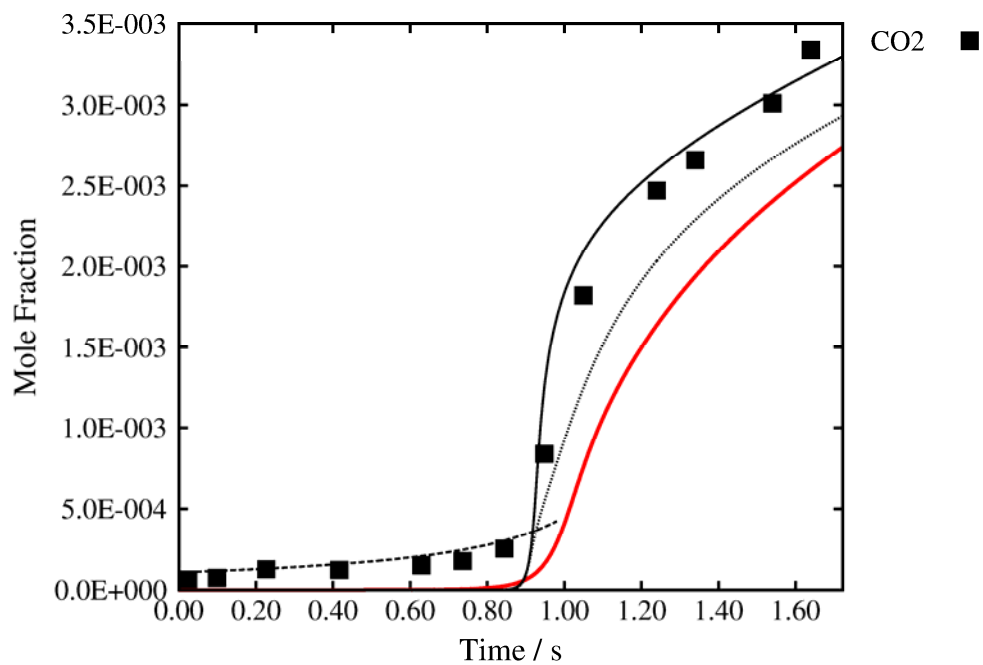
0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



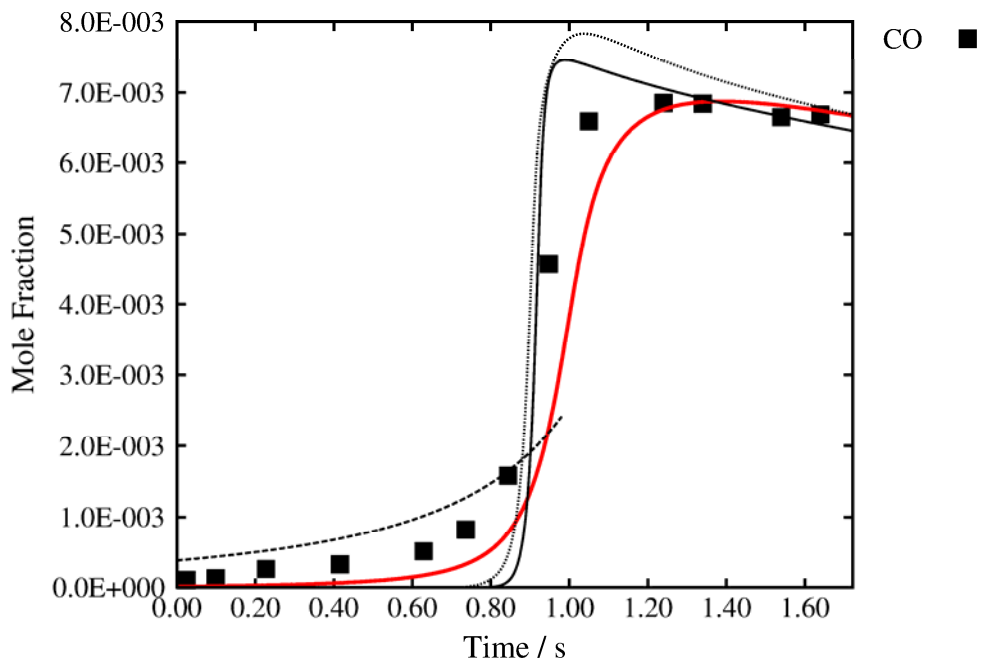
0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K



0.34% C₃H₆ 1.49% O₂ in N₂, $\Phi = 1.00$, $p = 12.5$ atm, $T = 861$ K

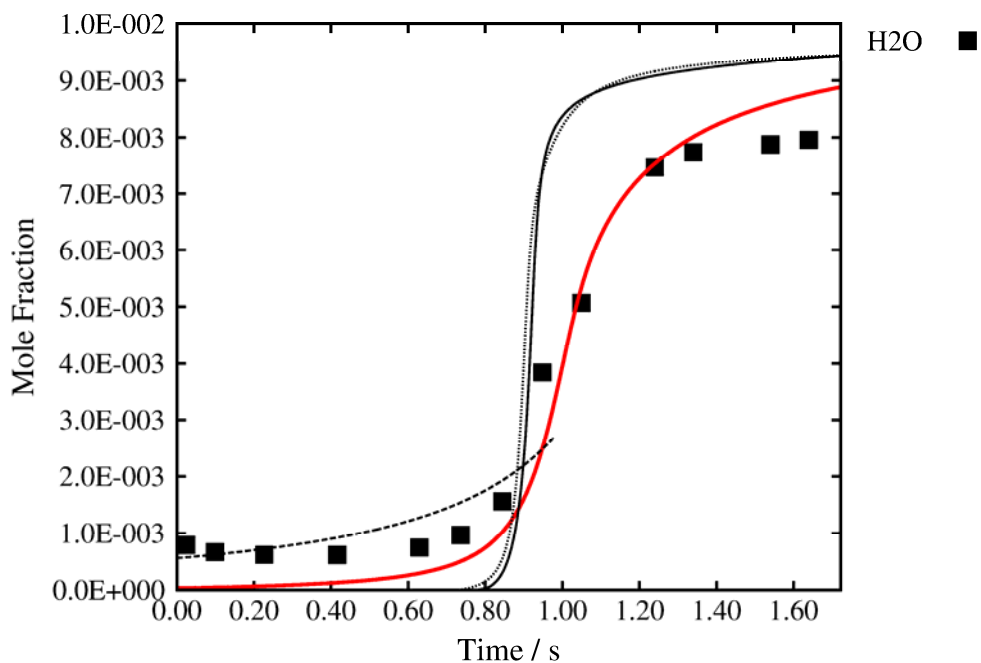
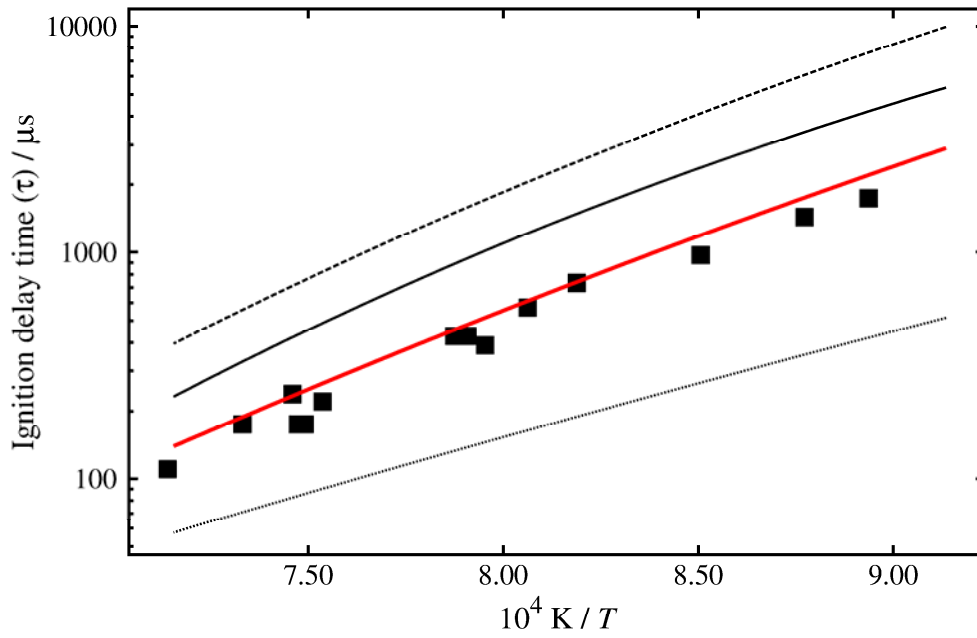
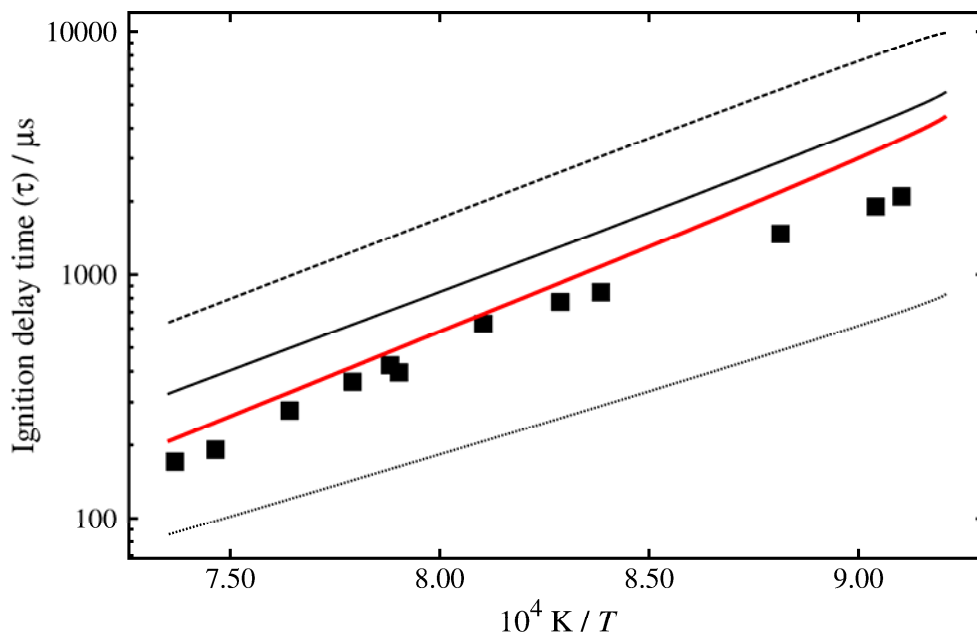


Figure 26 Flow reactor of propene/O₂/N₂. Symbols are experimental data (this study) lines are model predictions, time shifted to match 50% fuel consumed. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

4.46% C_3H_6 , in Air, $\Phi = 1.0$, $p_{av} = 10$ atm



2.281% C_3H_6 , in Air, $\Phi = 0.5$, $p_{av} = 10$ atm



0.89% C₃H₆, 4% O₂, in Ar, $\Phi = 1.0$, $p_{av} = 40$ atm

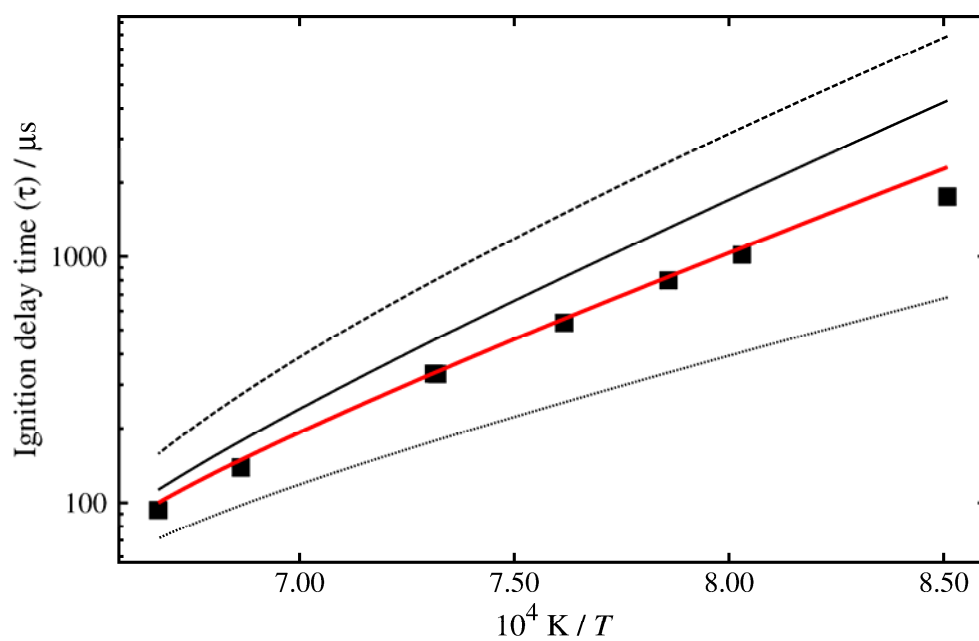
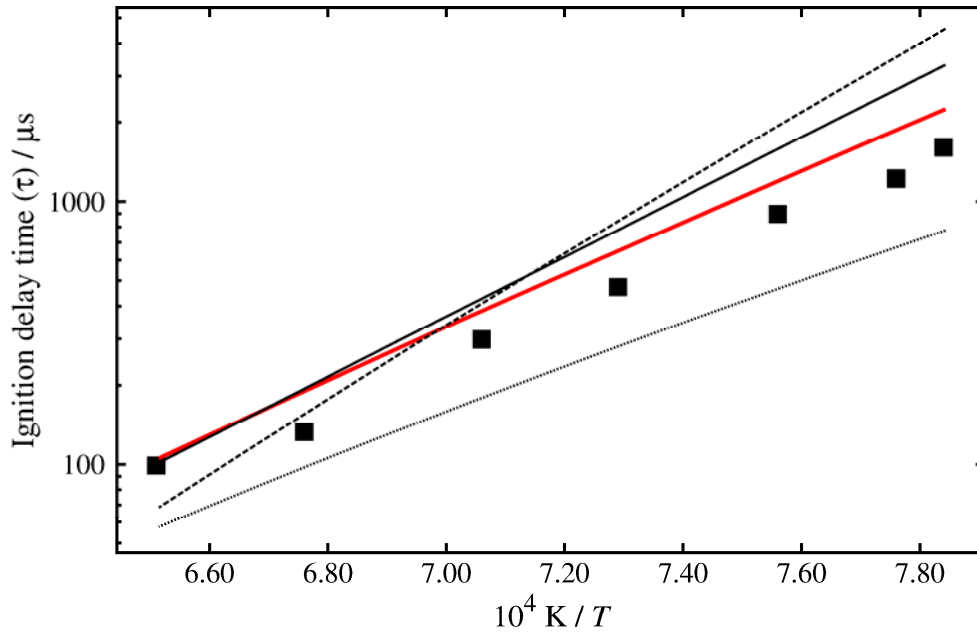
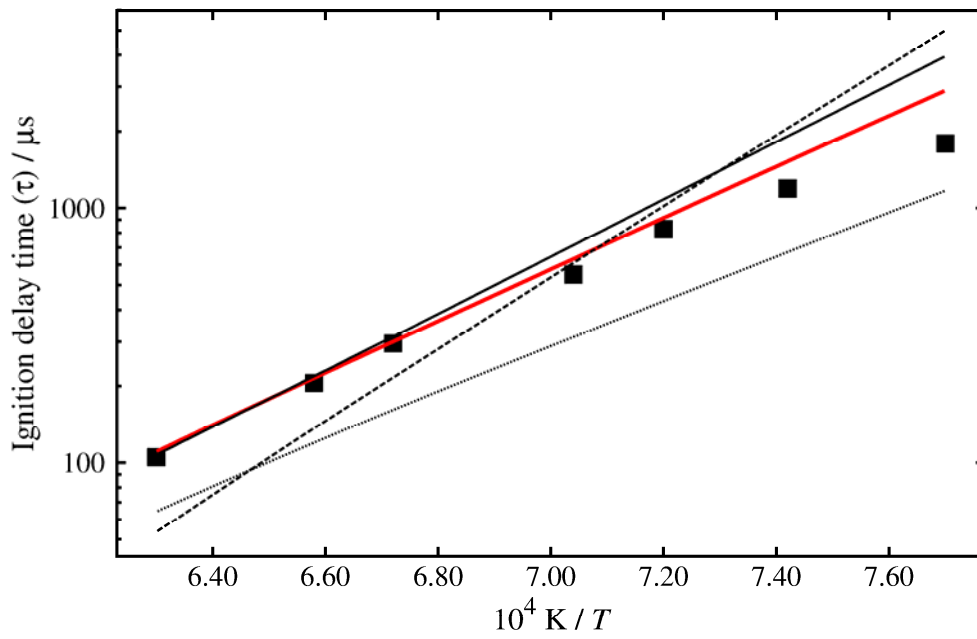


Figure 27 Shock tube ignition delay times of propene/O₂/Ar. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

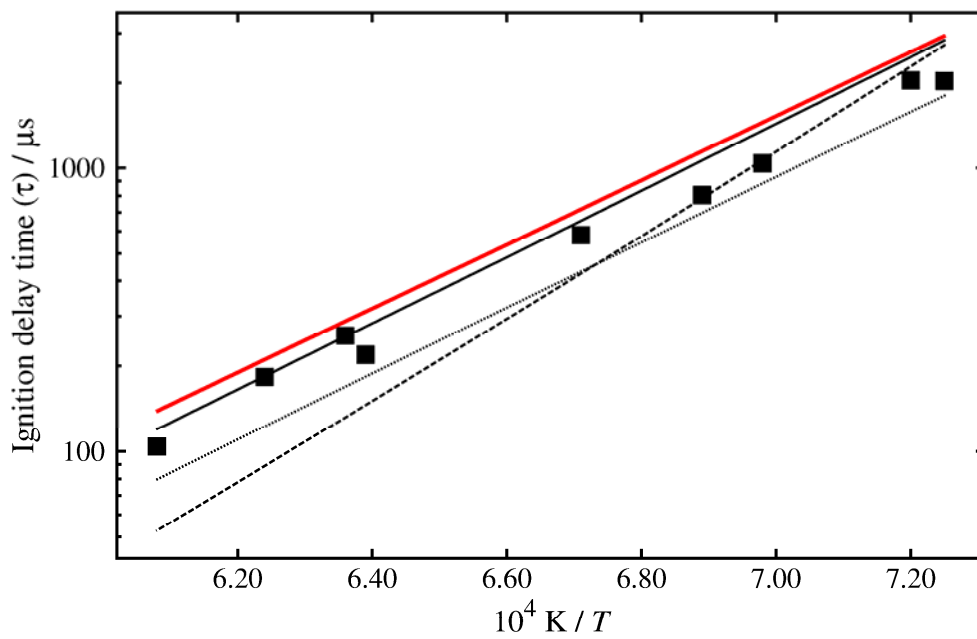
2.281% C₃H₆, in Air, $\Phi = 0.5$, $p_{av} = 2$ atm



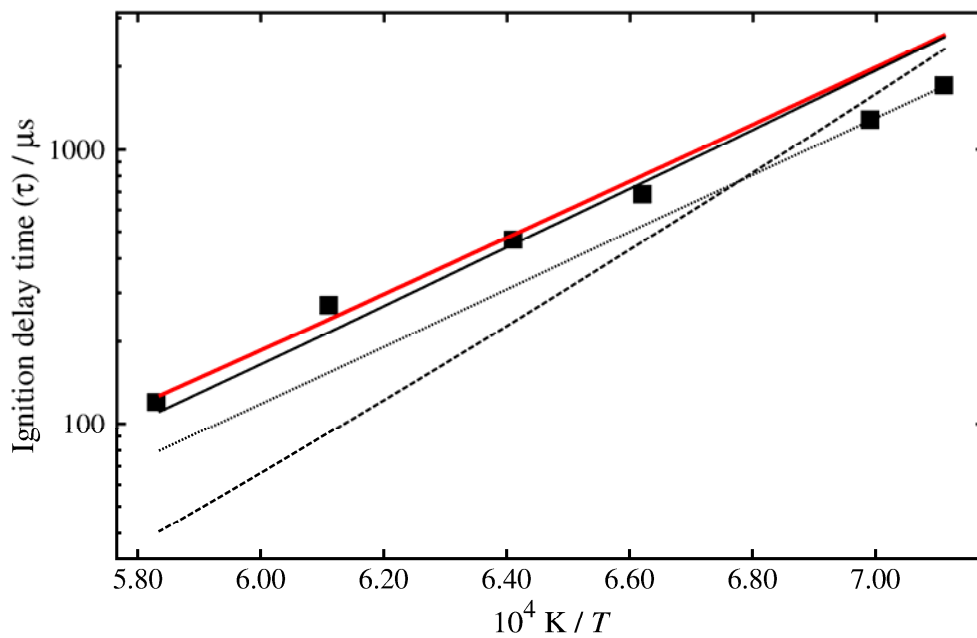
2.67% C₃H₆, 12.00% O₂ in Ar, $\Phi = 1.0$, $p_{av} = 2$ atm



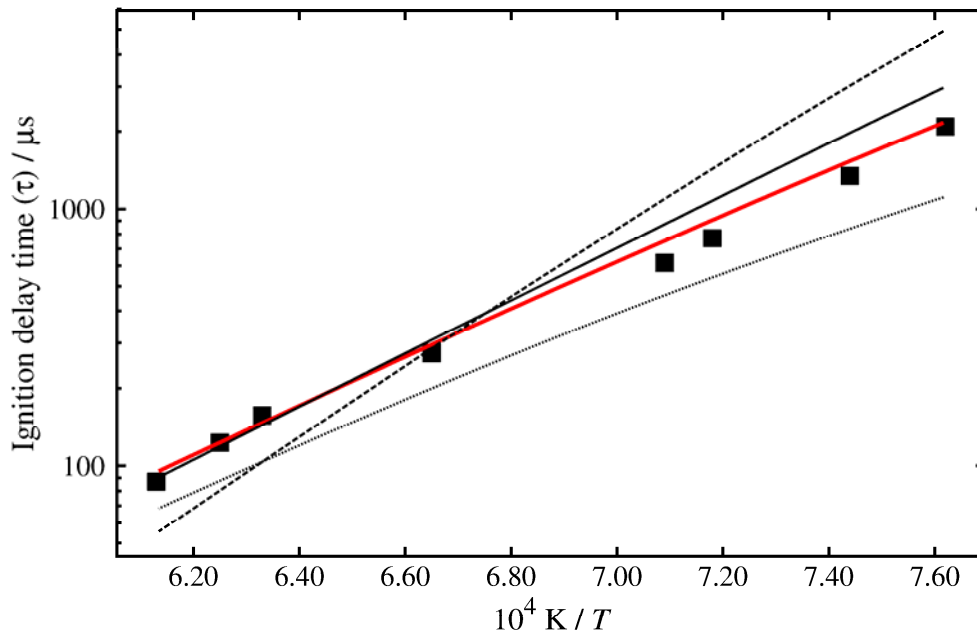
2.67% C₃H₆, 4.00% O₂ in Ar, $\Phi = 1.0$, $p_{av} = 2$ atm



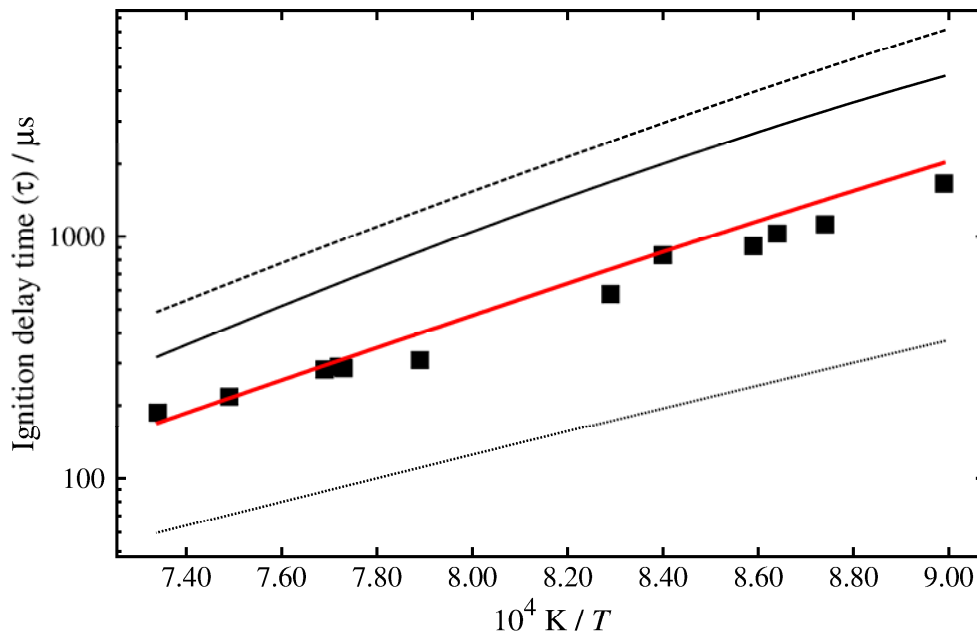
1.78% C₃H₆, 4.00% O₂ in Ar, $\Phi = 2.0$, $p_{av} = 2$ atm



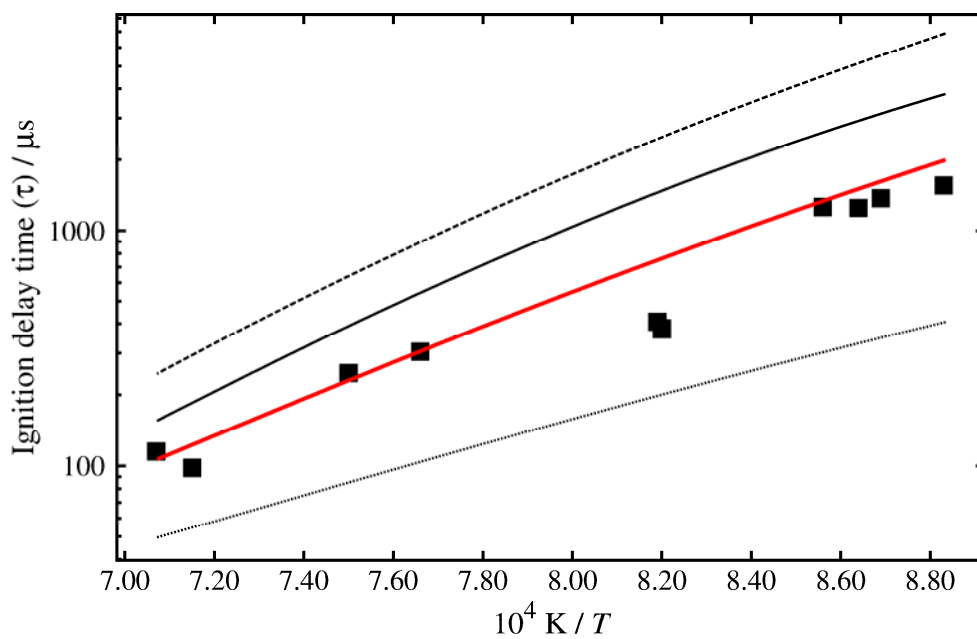
1.778% C₃H₆, in Air, $\Phi = 2.0$, $p_{av} = 10$ atm



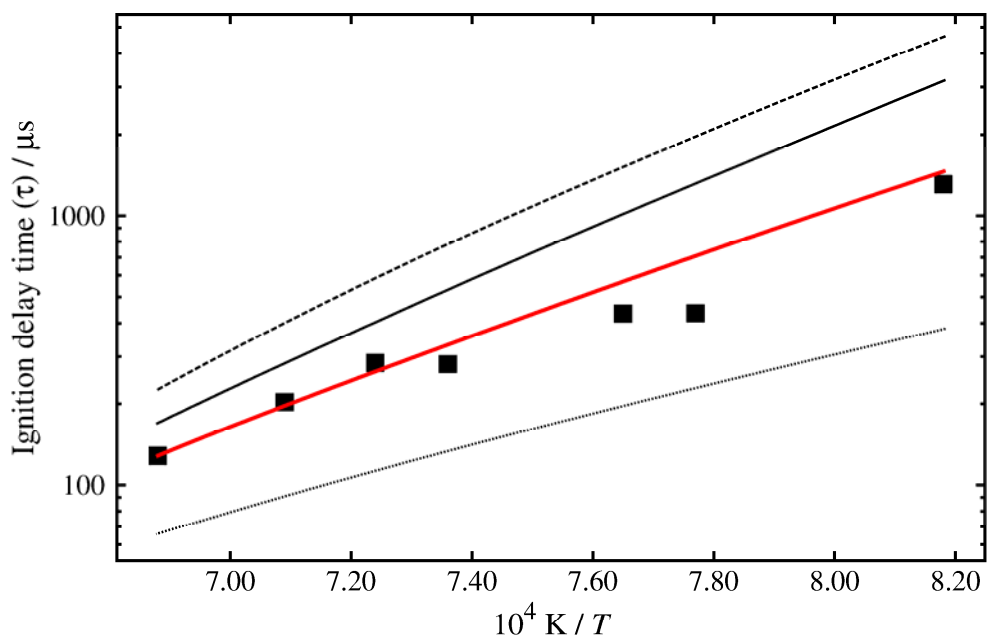
4.46% C₃H₆, in Air, $\Phi = 1.0$, $p_{av} = 10$ atm



2.281% C₃H₆, in Air, $\Phi = 0.5$, $p_{av} = 10$ atm



2.67% C₃H₆, 12.00% O₂ in Ar, $\Phi = 1.0$, $p_{av} = 10$ atm



0.889% C₃H₆, 4.00% O₂ in Ar $\Phi = 1.0$, $p_{av} = 10$ atm

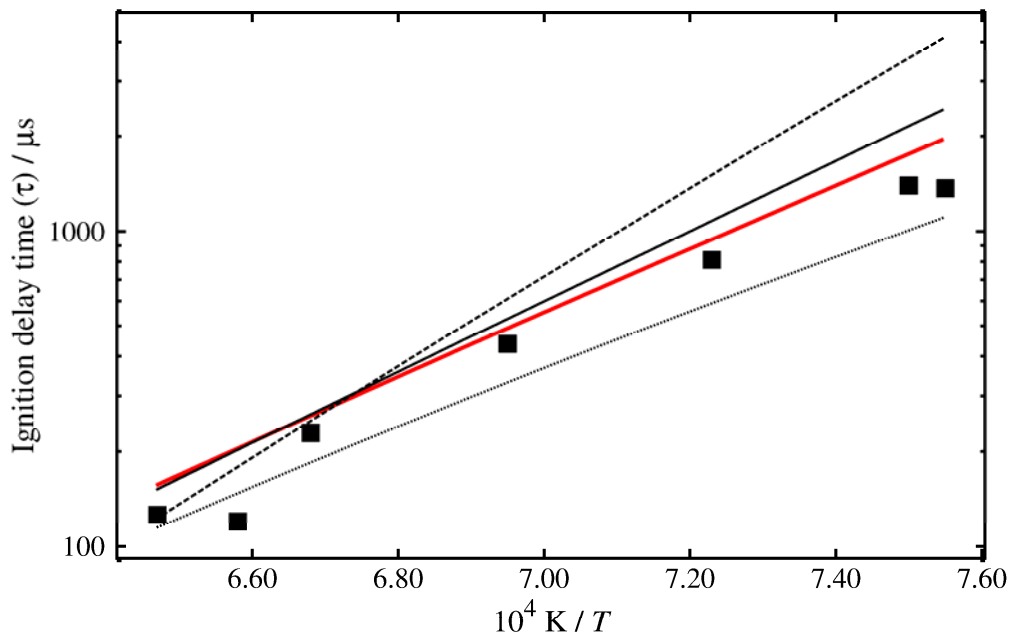
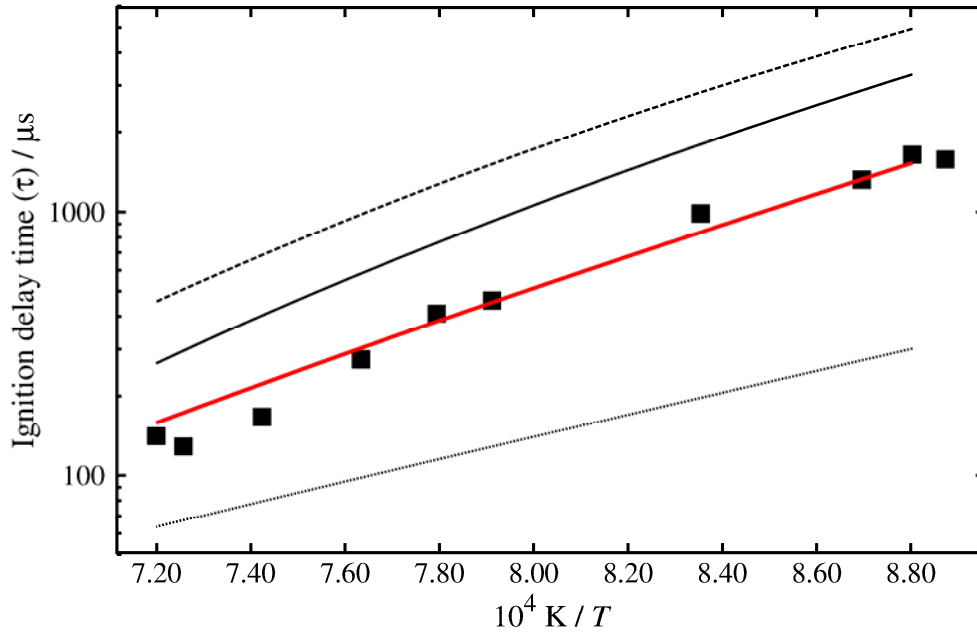
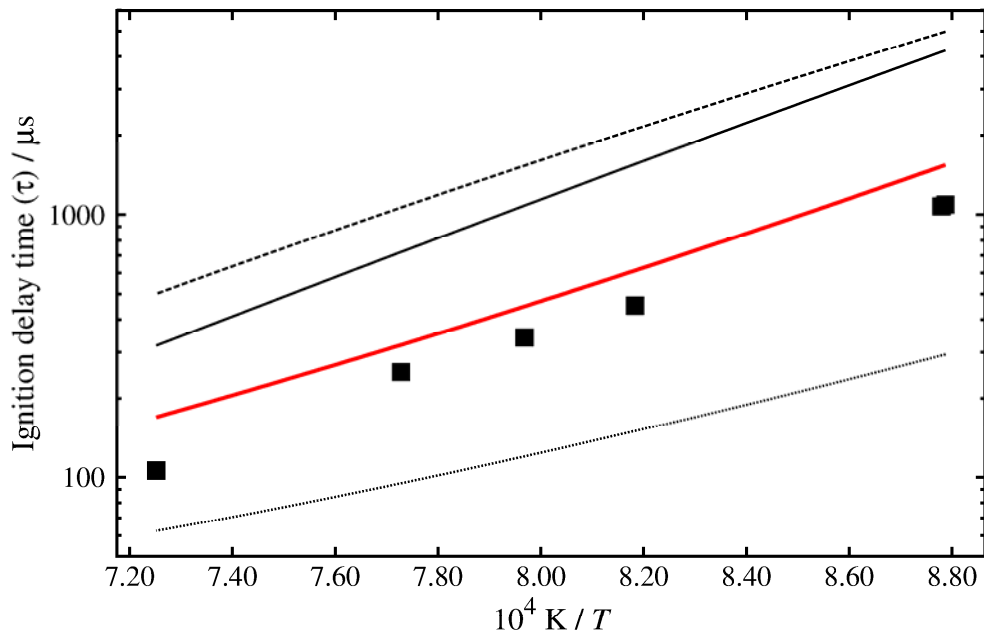
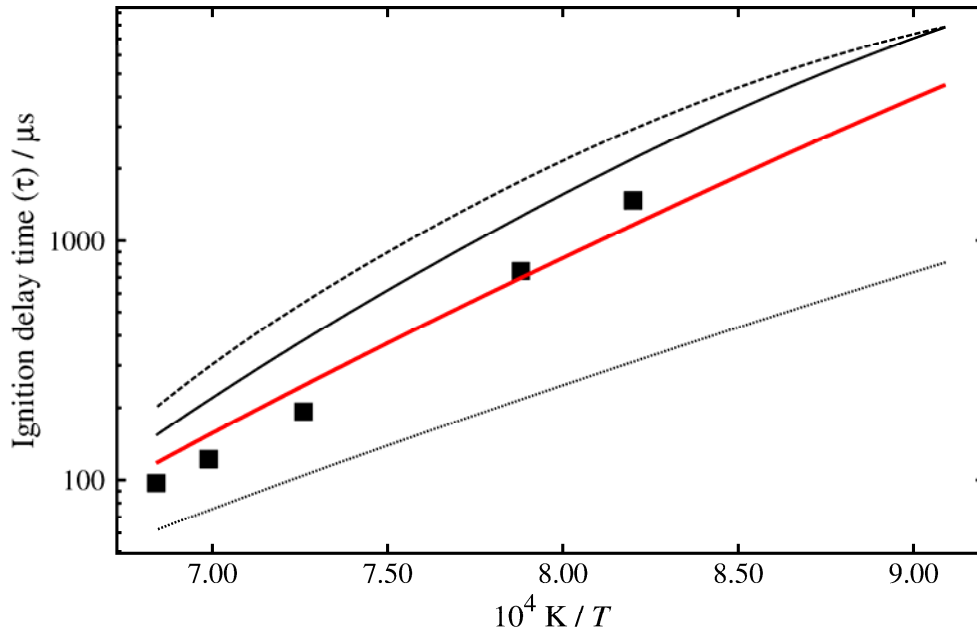


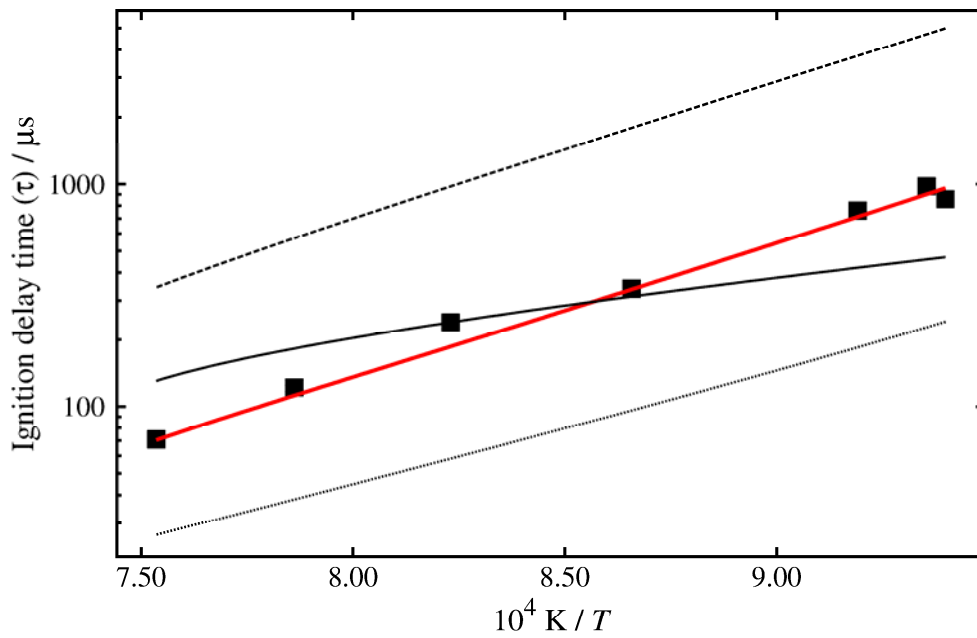
Figure 28 Shock tube ignition delay times of propene/O₂/Ar. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

4.46% C₃H₆, in Air, $\Phi = 1.0$, $p_{av} = 10$ atm8.54% C₃H₆, in Air, $\Phi = 2.0$, $p_{av} = 10$ atm

2.281% C₃H₆, in Air, $\Phi = 0.5$, $p_{av} = 10$ atm



2.281% C₃H₆, in Air, $\Phi = 0.5$, $p_{av} = 40$ atm



8.54% C₃H₆, in Air, $\Phi = 2.0$, $p_{av} = 40$ atm

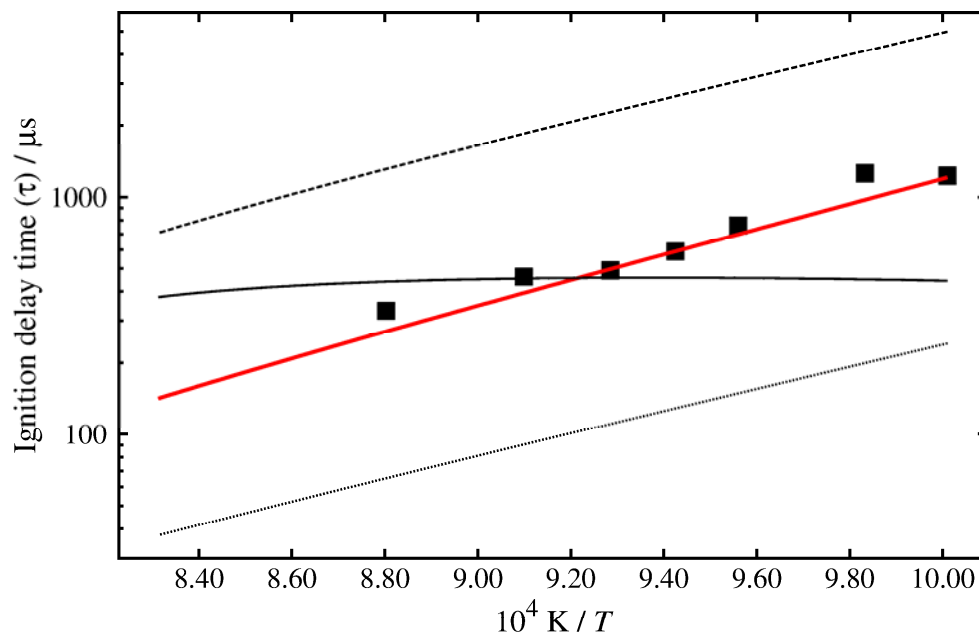
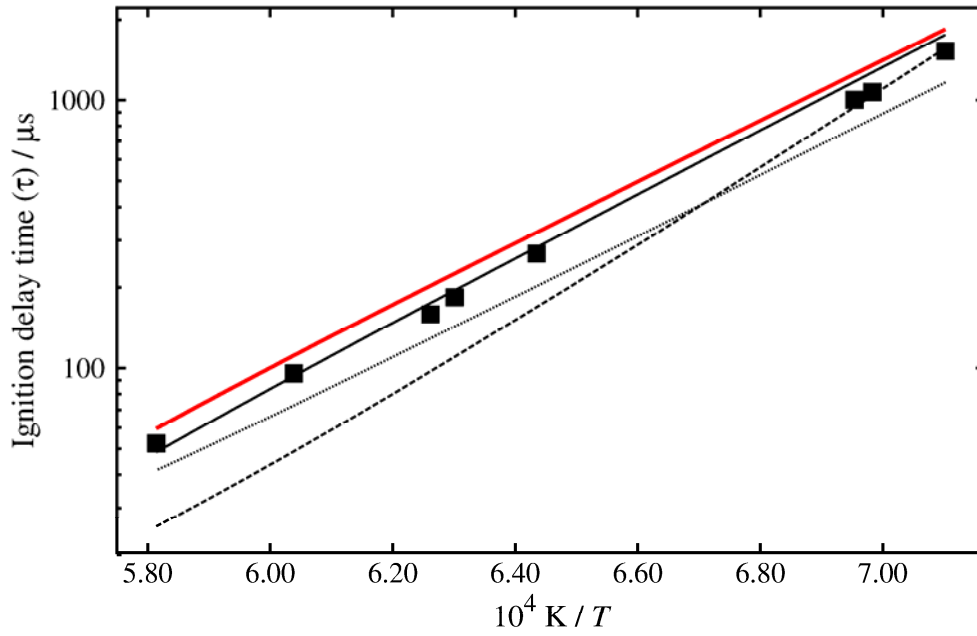


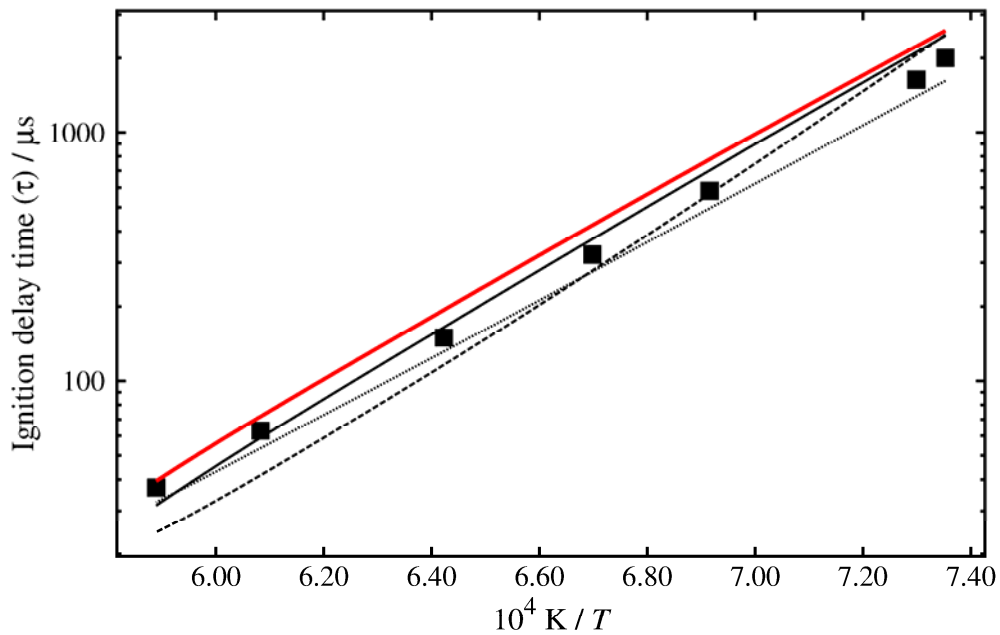
Figure 29 Shock tube ignition delay times of propene/Air. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

Stanford

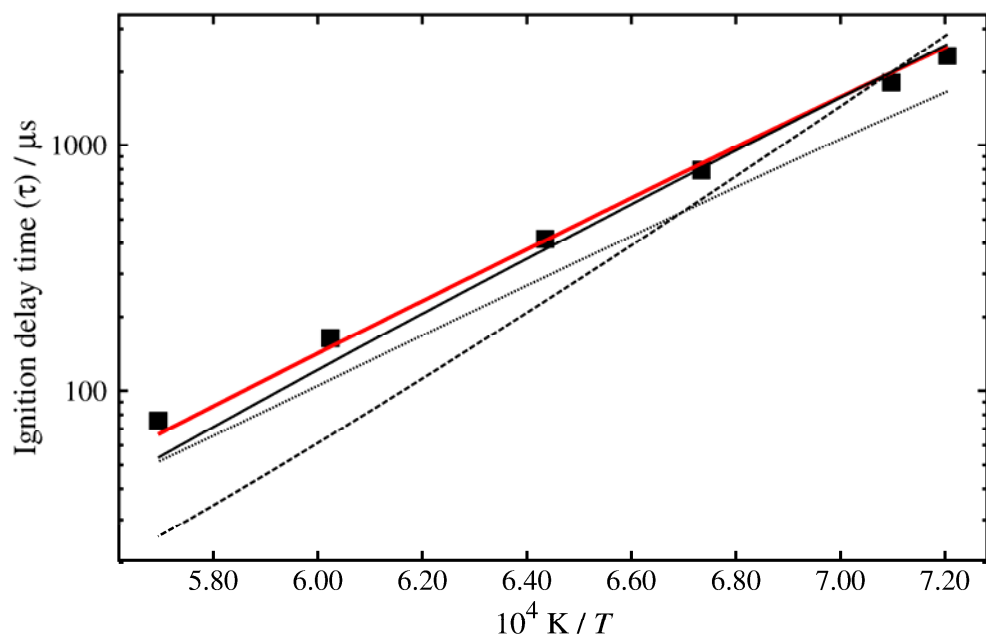
0.88% C₃H₆, 4.00% O₂ 95.12% Ar, $\Phi = 1.0$, $p_{av} = 2.07$ atm



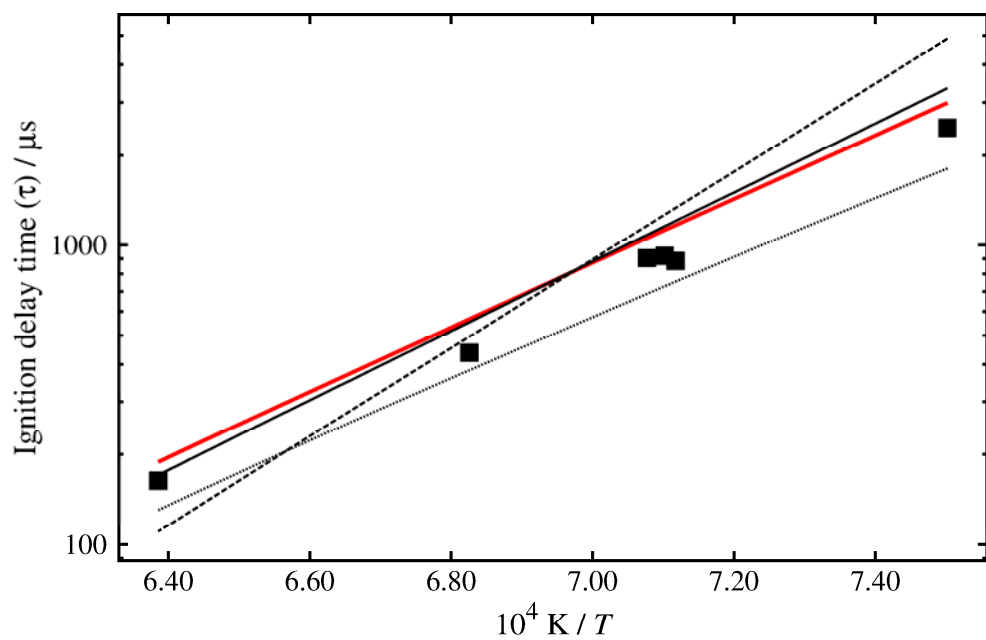
0.40% C₃H₆, 4.00% O₂ 95.56% Ar, $\Phi = 0.5$, $p_{av} = 2.32$ atm



1.80% C₃H₆, 4.00% O₂ 94.22% Ar, $\Phi = 2.0$, $p_{av} = 2.07$ atm



0.88% C₃H₆, 4.00% O₂ 95.12% Ar, $\Phi = 1.0$, $p_{av} = 4.50$ atm



1.67% C₃H₆, 7.20% O₂, 99.91% Ar, $\Phi = 1.0$, $p_{av} = 4.33$ atm

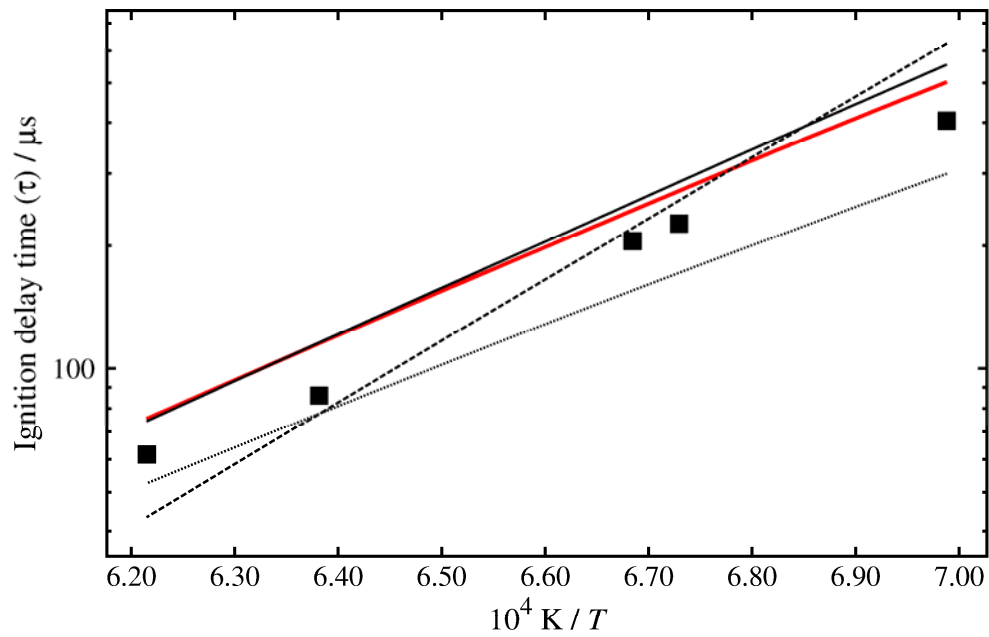
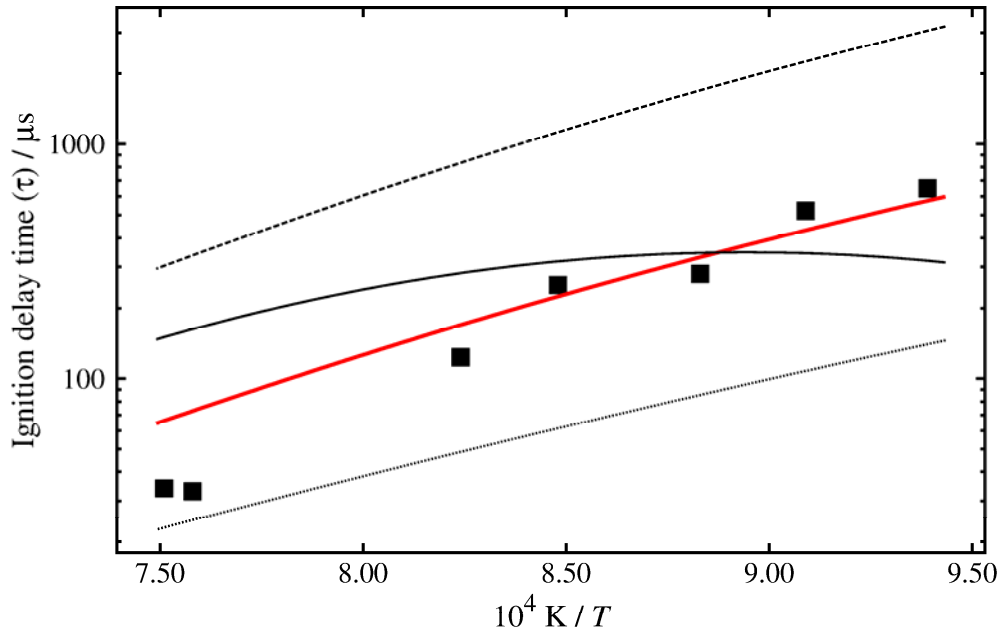
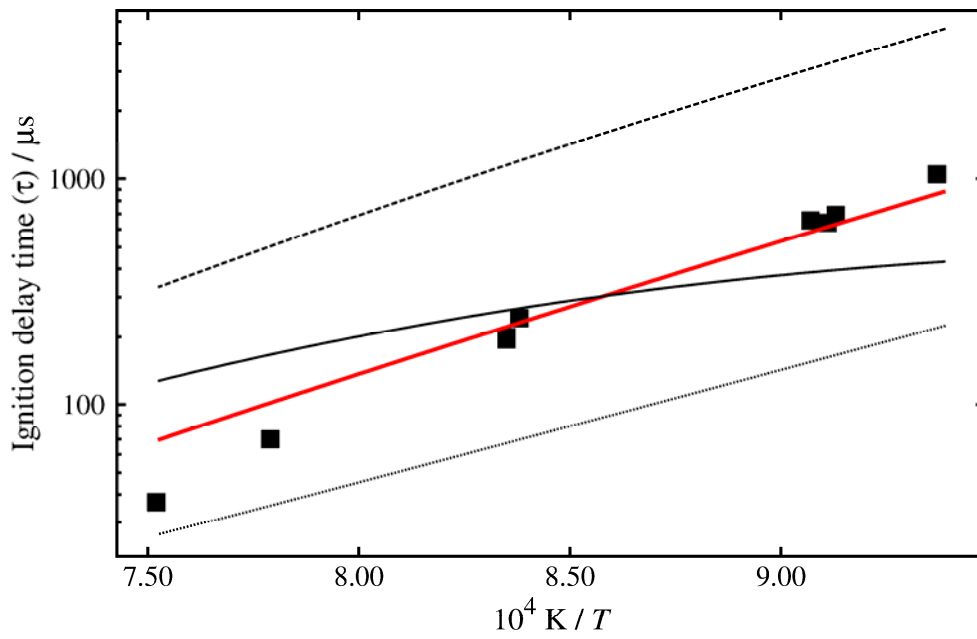


Figure 30 Shock tube ignition delay times of propene/O₂/Ar. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

4.46% C₃H₆, in Air, $\Phi = 1.0$, $p_{av} = 40$ atm



2.281% C₃H₆, in Air, $\Phi = 0.5$, $p_{av} = 40$ atm



8.54% C₃H₆, in Air, $\Phi = 2.0$, $p_{av} = 40$ atm

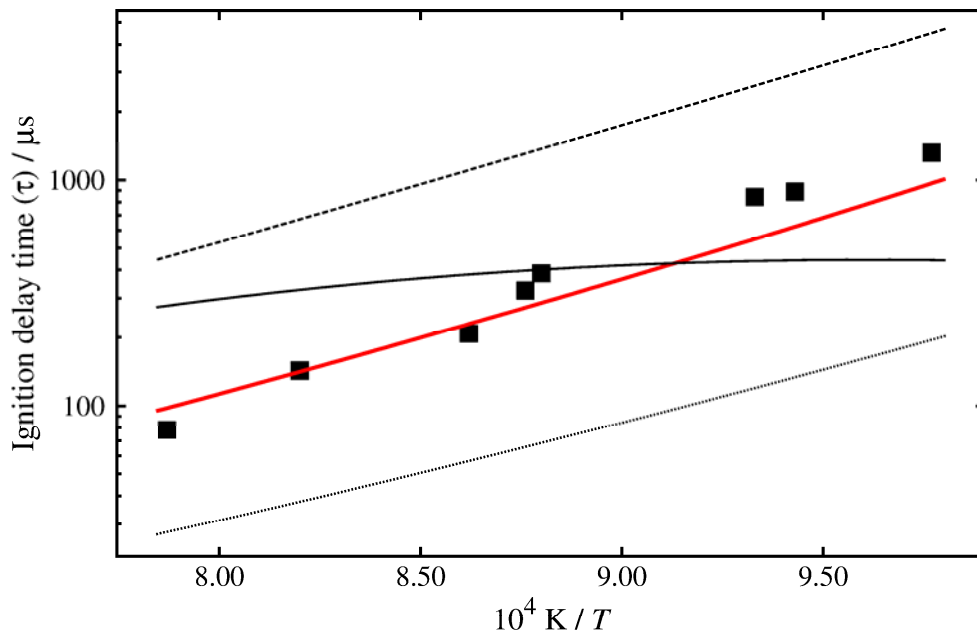


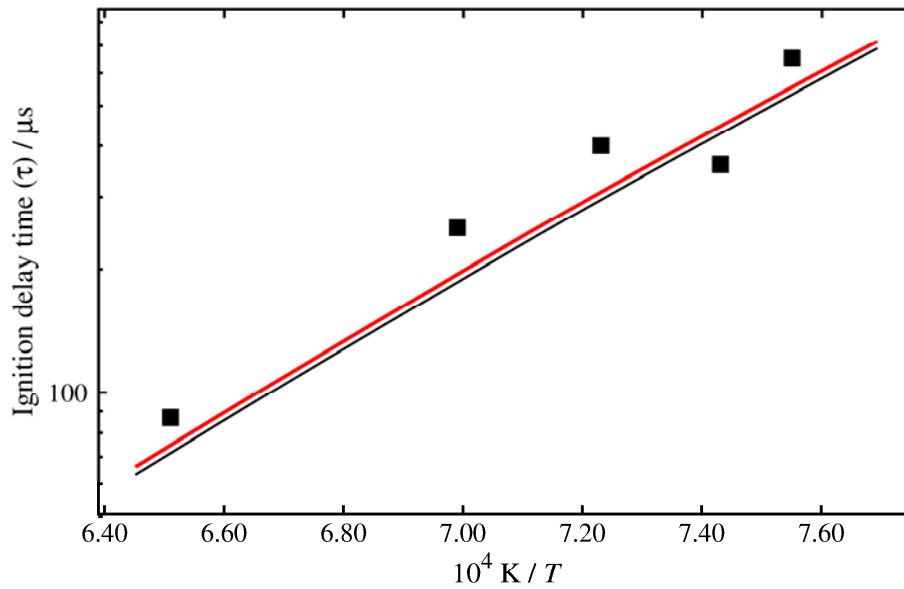
Figure 31 Shock tube ignition delay times of propene/Air. Symbols are experimental data (this study) lines are model predictions. — AramcoMech 2.0, — AramcoMech 1.3 [1], - - - Heyberger et al. [2], ••• USC II[3].

Performance of AramcoMech 2.0 on C₁–C₂ Targets

Mechanism performance against C₁–C₂ targets has changed very little from the performance of AramcoMech1.3 [1] as shown against selected targets below. Mechanism performance against ethylene targets has altered when compared to AramcoMech 1.3. The change in performance against the ethylene targets is due to the inclusion of the rate constant of $C_3H_6 + \dot{H} \rightleftharpoons C_2H_4 + \dot{C}H_3$ from Miller and Klippenstein [8], this is discussed in detail below.

**Methane
Shock tube**

20.0% CH₄, 13.3% O₂ 66.7% Ar, $\Phi = 3.0$, $p = 40.0$ atm



20.0% CH₄, 13.3% O₂ 66.7% Ar, $\Phi = 3.0$, $p = 115.0$ atm

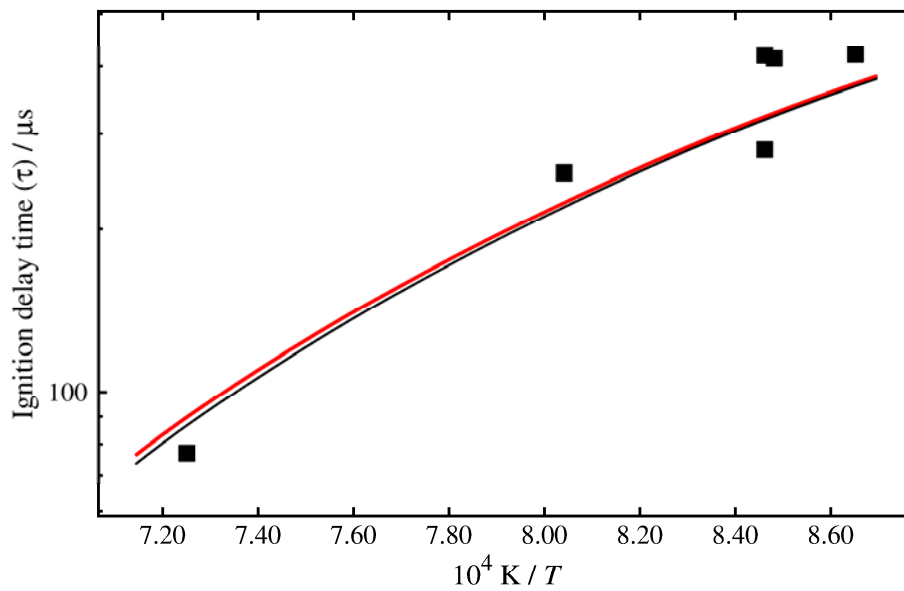


Figure 32 Shock tube ignition delay times of methane/oxygen/argon mixtures. Symbols are experimental data [9] lines are model predictions — current model — AramcoMech1.3.

Jet-stirred reactor

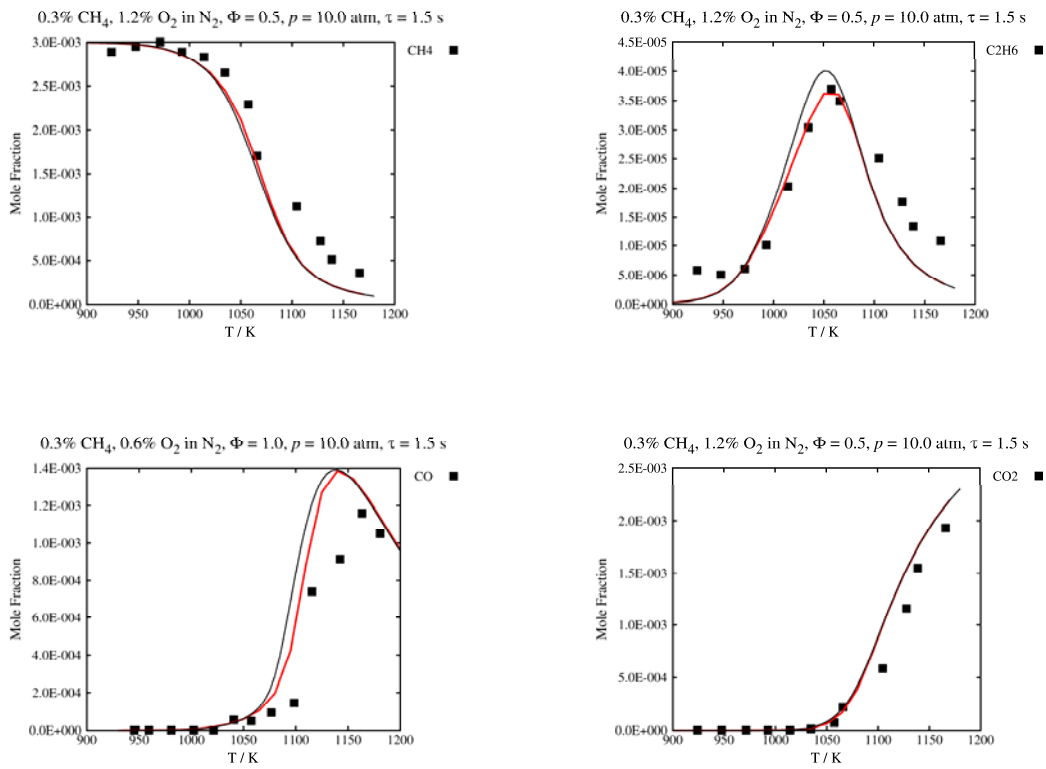


Figure 33 Jet-stirred reactor species profiles of methane/oxygen/nitrogen mixtures. Symbols are experimental data [10] lines are model predictions — red — current model — black — AramcoMech 1.3.

Ethane
Shock tube

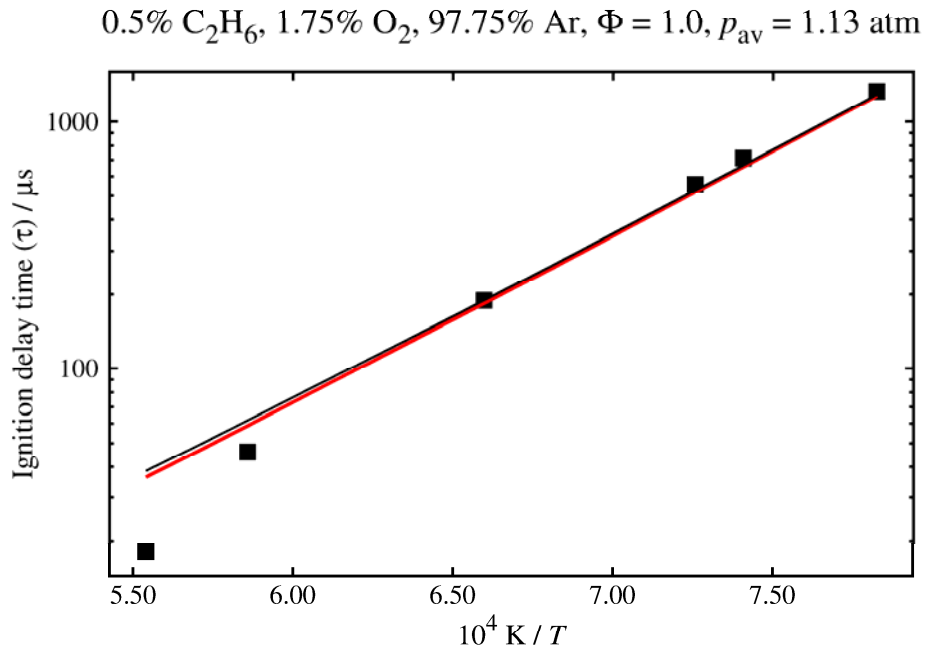
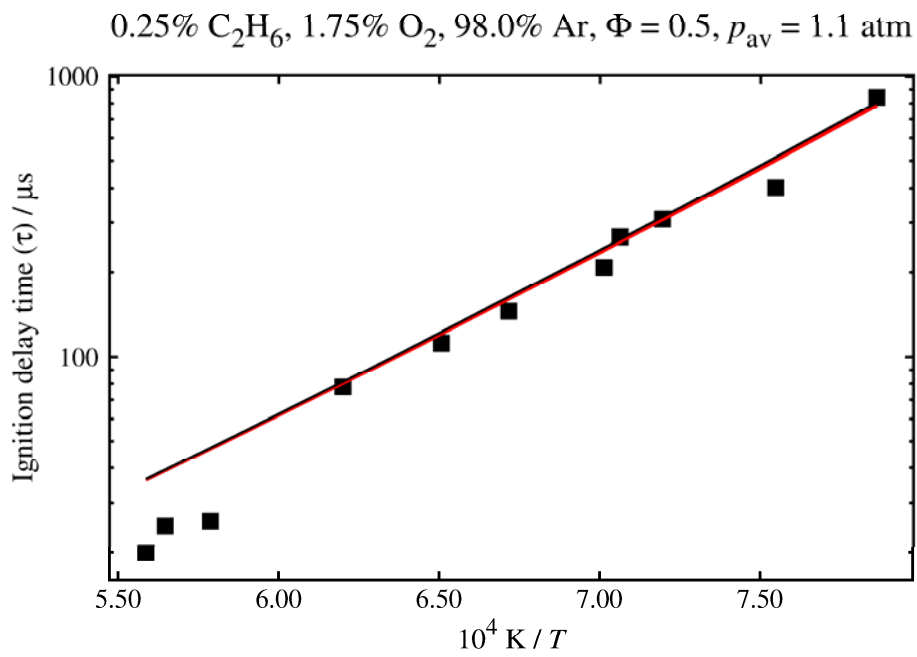


Figure 34 Shock tube ignition delay times of ethane/oxygen/argon mixtures.
Symbols are experimental data [11] lines are model predictions — current model —
AramcoMech 1.3.

Jet-stirred reactor

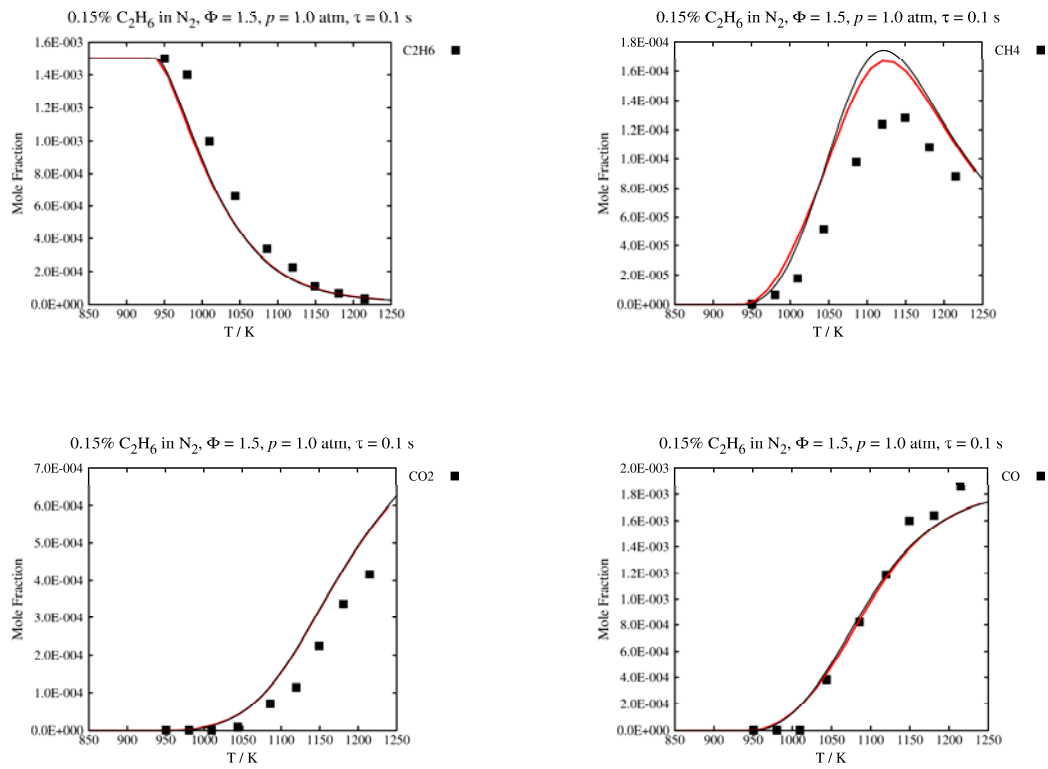


Figure 35 Jet-stirred reactor species profiles of ethane/oxygen/nitrogen mixtures. Symbols are experimental data [12] lines are model predictions — red — current model — black — AramcoMech 1.3.

*Ethylene
Shock tube*

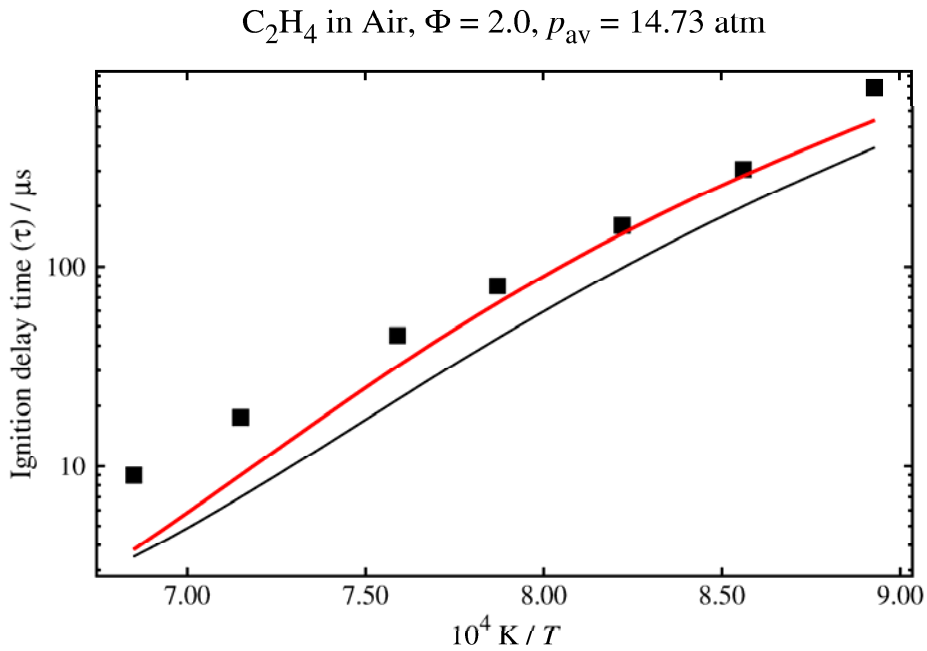
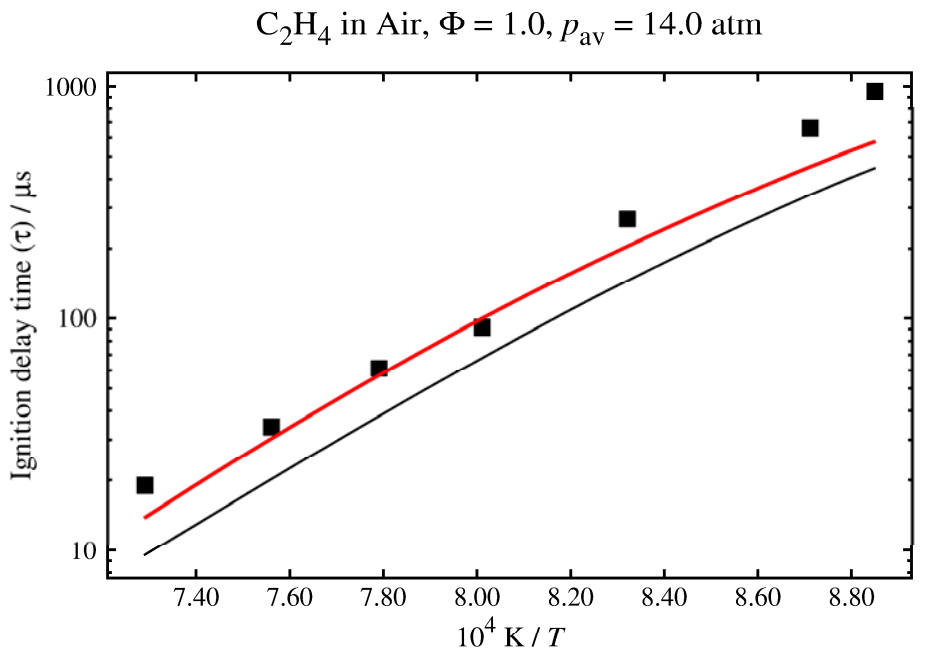


Figure 36 Shock tube ignition delay times of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [19] lines are model predictions. — current model — AramcoMech 1.3.

Jet-stirred reactor

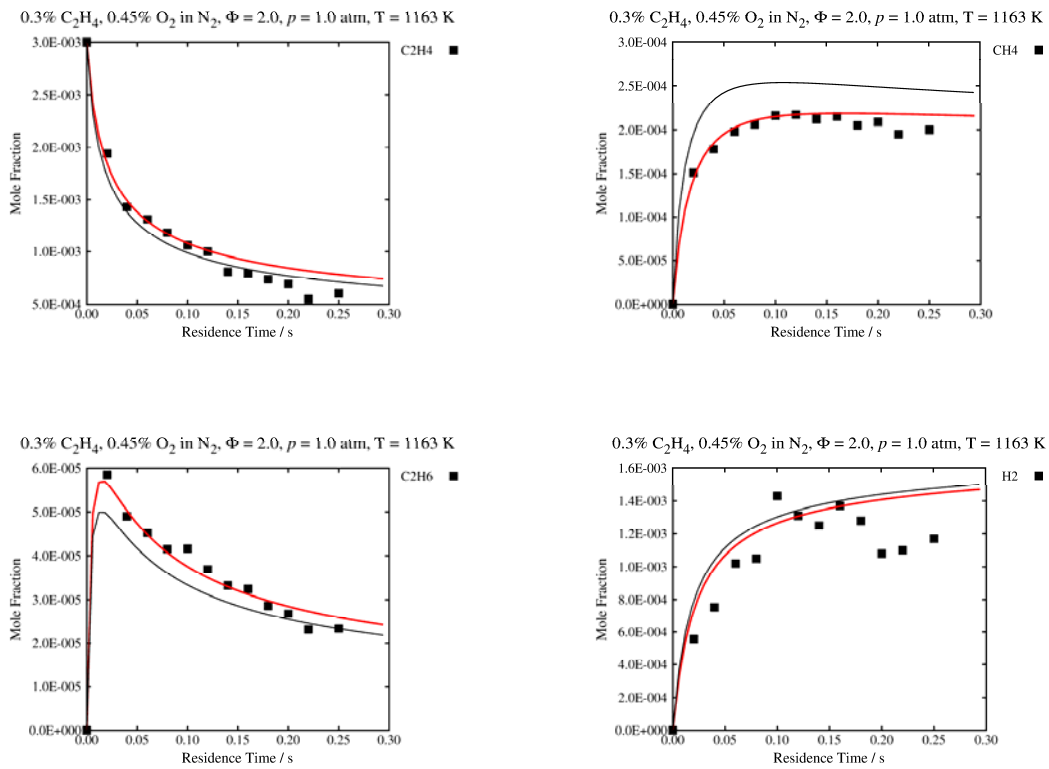
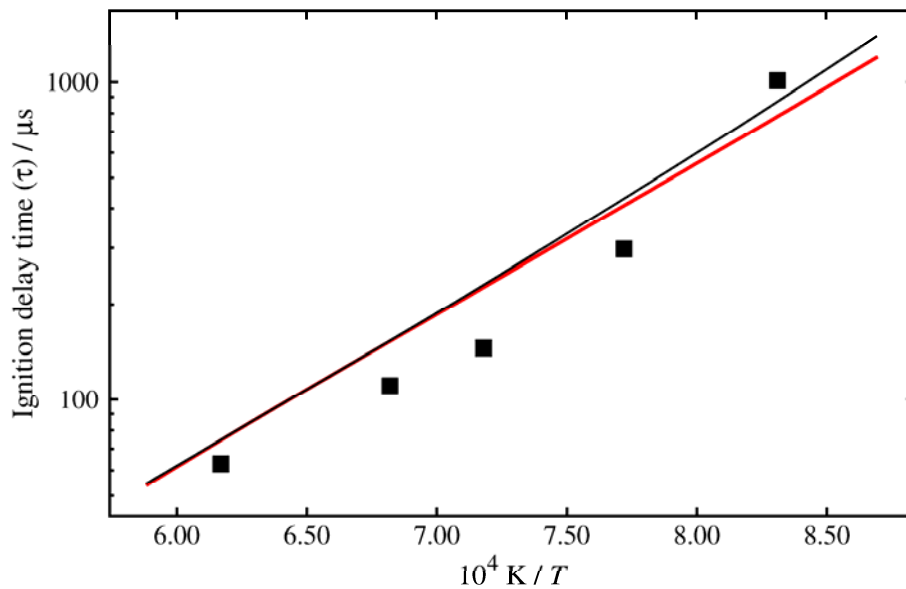


Figure 37 Jet-stirred reactor species profiles of ethylene/oxygen/nitrogen mixtures. Symbols are experimental data [13] lines are model predictions — current model — AramcoMech

*Acetylene
Shock tube*

0.5% C₂H₂, 1.25% O₂, 98.25% Ar, $\Phi = 1.0$, $p_{av} = 1.85$ atm



0.5% C₂H₂, 2.54% O₂, 96.96% Ar, $\Phi = 0.49$, $p_{av} = 1.85$ atm

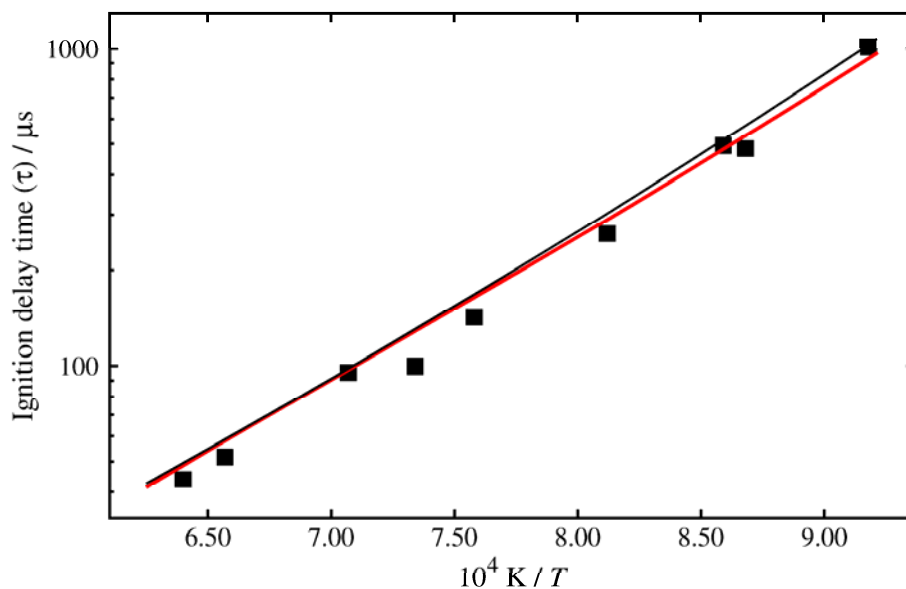
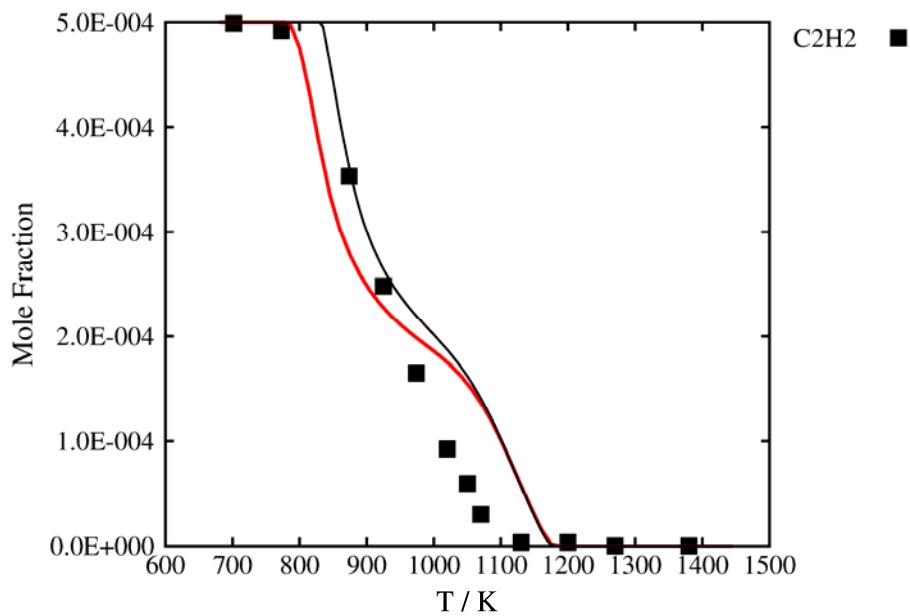


Figure 38 Shock tube ignition delay times of acetylene/oxygen/argon mixtures. Symbols are experimental data [14] lines are model predictions.— red — current model — black — AramcoMech 1.3.

Flow reactor

500 ppm C_2H_2 , 0.7% H_2O , in N_2 , $\Phi = 1.43$, $p = 1.0$ atm, $\tau = 195/T$ s



500 ppm C_2H_2 , 0.7% H_2O , in N_2 , $\Phi = 1.43$, $p = 1.0$ atm, $\tau = 195/T$ s

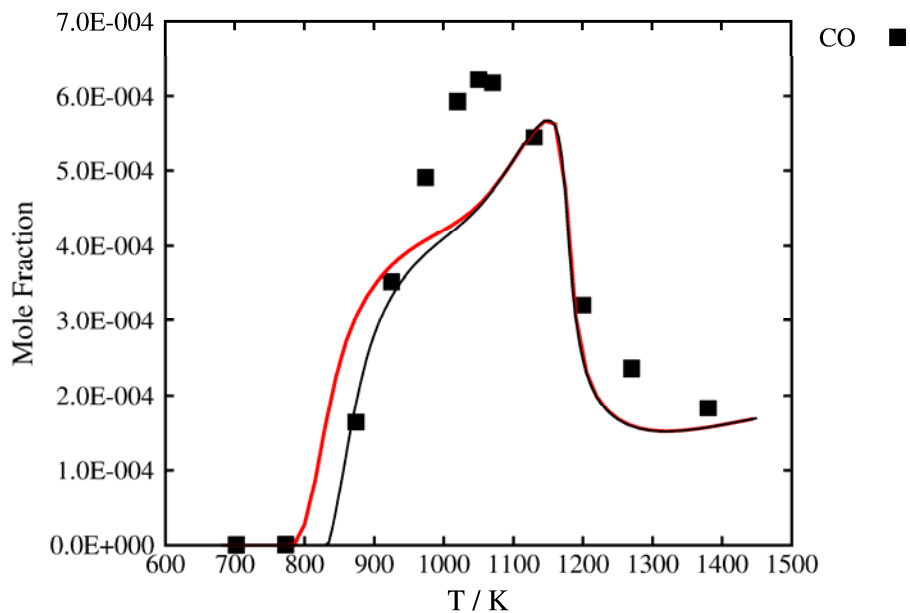
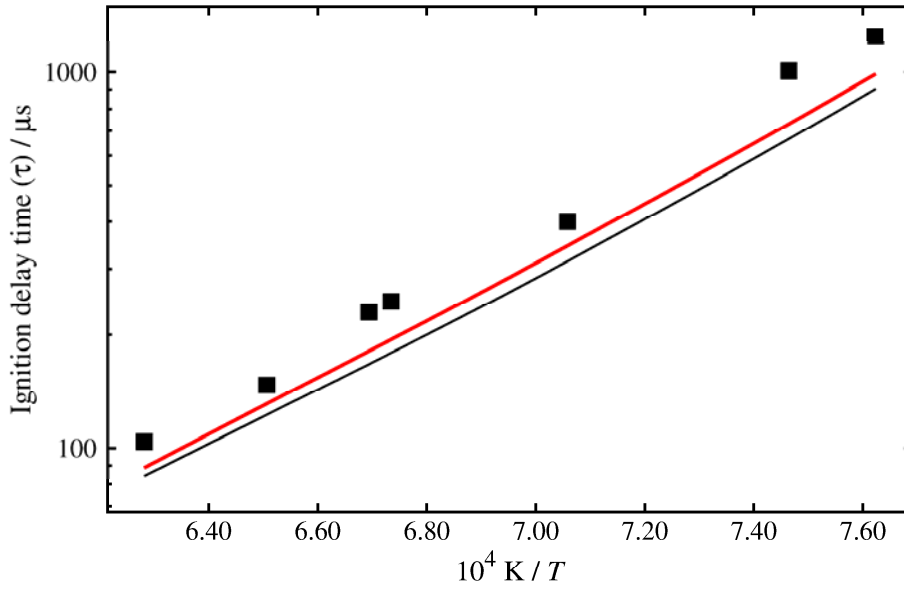


Figure 39 Flow reactor species profiles of acetylene/oxygen/water/nitrogen mixtures. Symbols are experimental data [15] lines are model predictions — red — current model — black — AramcoMech 1.3.

**Methane/Ethane
Shock tube**

5.56% CH₄, 1.85% C₂H₆, 17.59% O₂, 75.0% Ar, $\Phi = 1.0$, $p = 1.0$ atm



1.11% CH₄, 0.37% C₂H₆, 3.52% O₂, 95.0% Ar, $\Phi = 1.0$, $p = 10.0$ atm

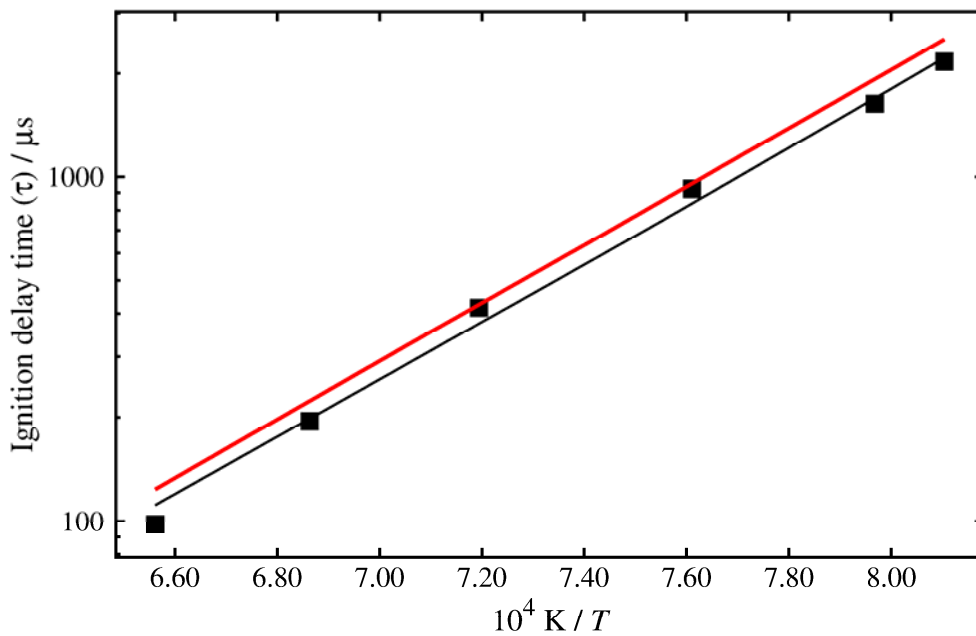


Figure 40 Shock tube ignition delay times of methane/ethane/oxygen/argon mixtures. Symbols are experimental data [16] lines are model predictions. — red — current model — black — AramcoMech 1.3.

Jet-stirred reactor

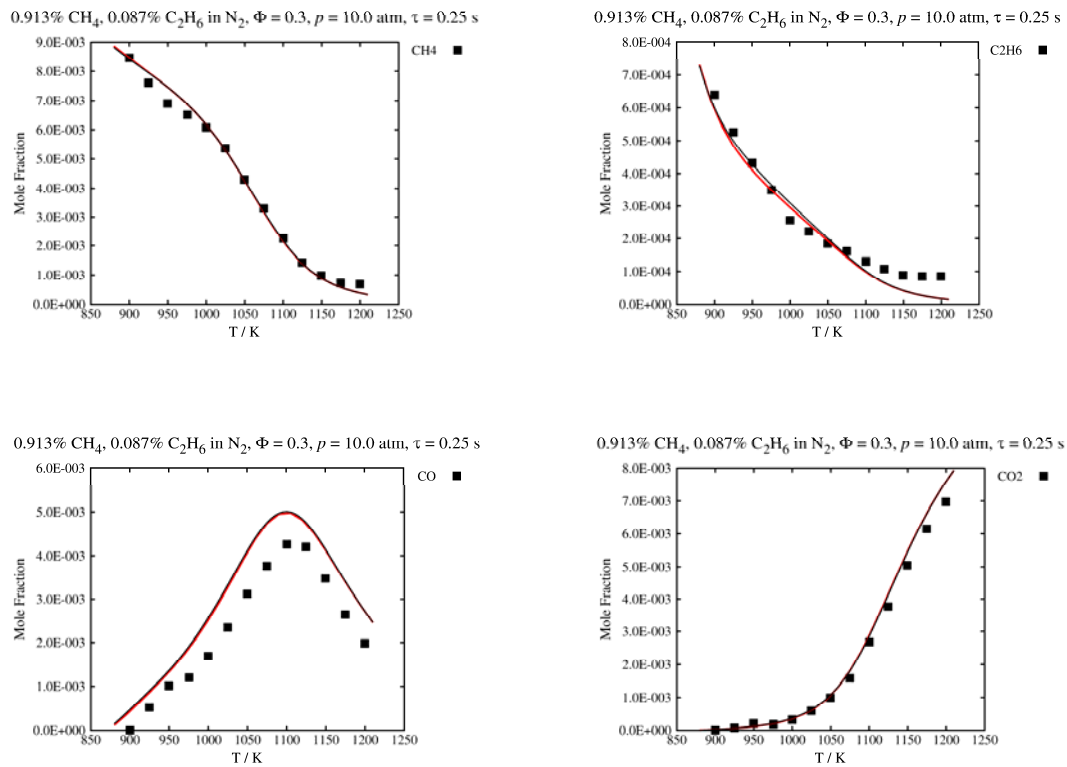


Figure 41 Jet-stirred reactor species profiles of methane/ethane/oxygen/nitrogen mixtures. Symbols are experimental data [16] lines are model predictions — current model — AramcoMech

Ethylene

Kopp *et al.* [18]

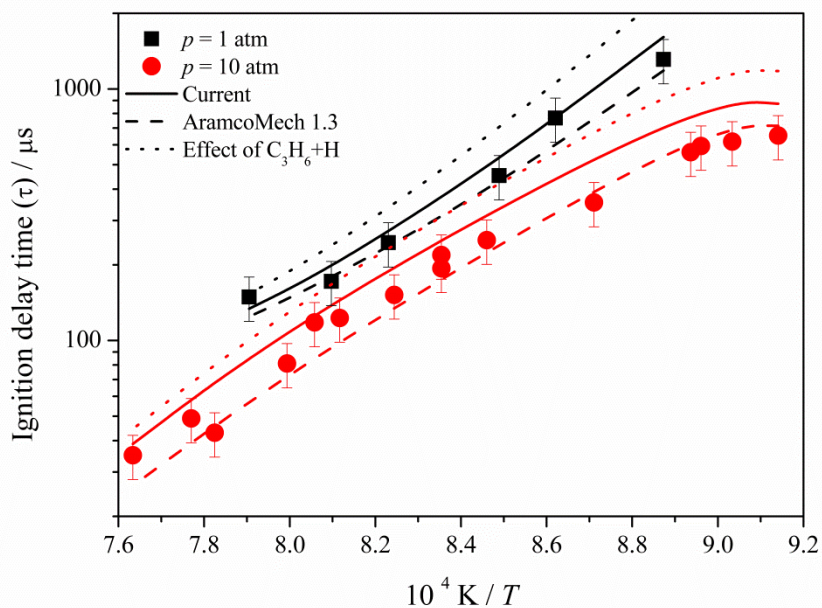


Figure 42 Shock tube ignition delay times of ethylene/Air at $\phi = 1.0$. Symbols are experimental data [18] with 20% error bars, lines are model predictions.

Penyazkov *et al.* [19]

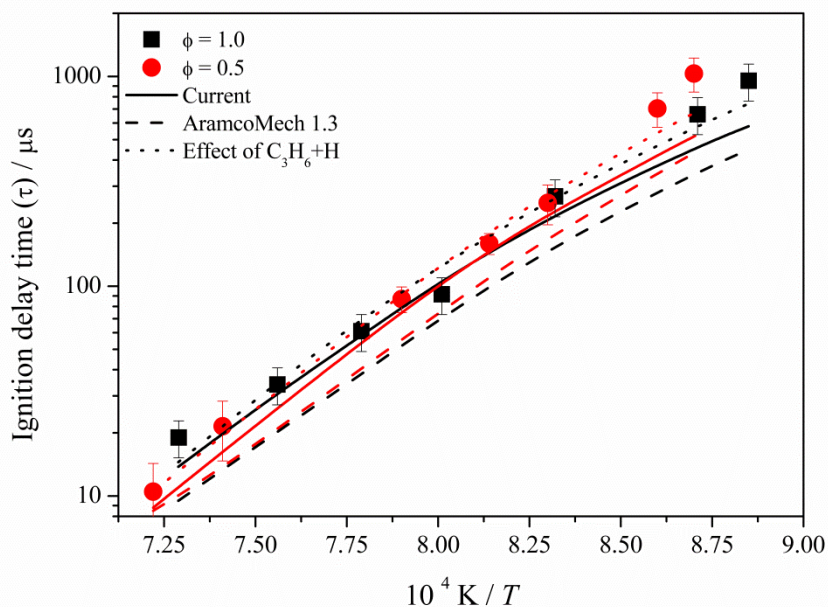


Figure 43 Shock tube ignition delay times of ethylene/Air at $p = 14$ atm. Symbols are experimental data [19] with 20% error bars, lines are model predictions.

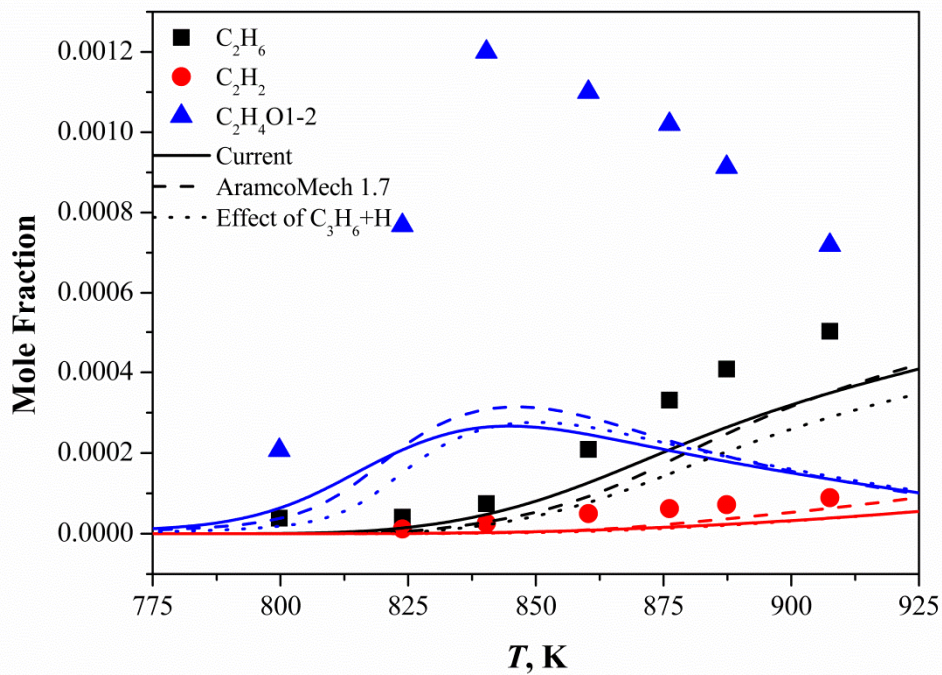
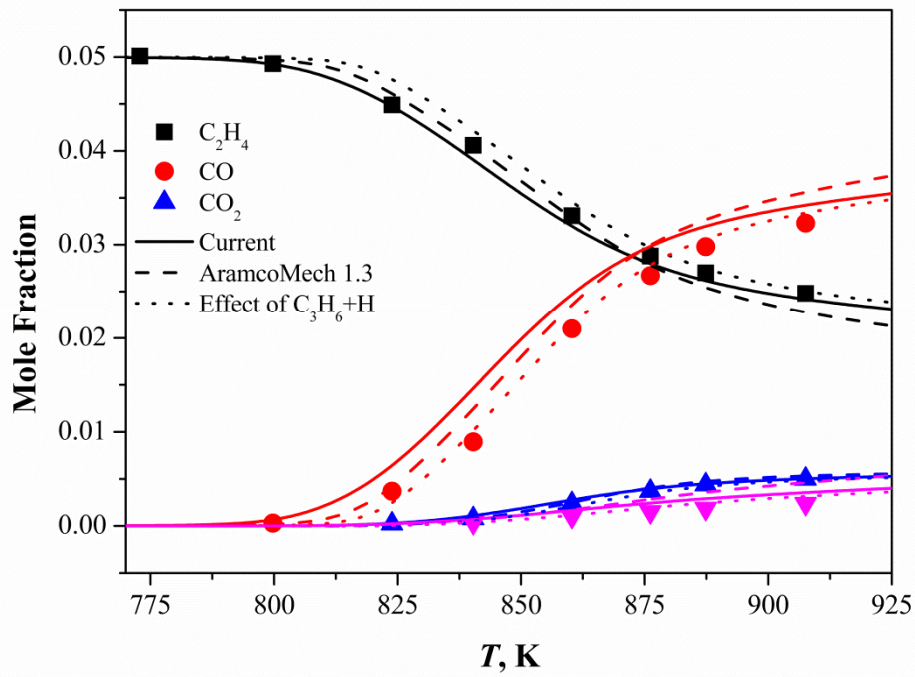


Figure 44 Jet-stirred reactor for 5 % C₂H₄/ in N₂, $\phi = 3.0$, $p = 1.0$ atm. Symbols are experimental data [20] lines are model predictions.

Inclusion of the Miller and Klippenstein rate constants resulted in a reduction in reactivity as shown in Figs. 42–44. Predicted ignition delay times for fuel in air mixtures at $\phi = 1$ at pressures of 1 and 10 atm were significantly slower using the Miller and Klippenstein recommendation than the experimental measurements from Kopp et al. (dashed line Fig. 42). In order to improve the mechanism performance an alteration to the branching ratio of the reaction of the vinyl radical with molecular oxygen. In AramcoMech 1.3 the crossover over temperature between chain-branching and chain-propagating occurred at approximately 1000K, in the current mechanism the cross over occurs at approximately 900K, Fig 45. The current mechanism shows relatively good agreement with ethylene targets across a range of conditions and shows improved performance in comparison to AramcoMech 1.3 against the ignition delay times of Penyazkov et al. [19], Fig. 43.

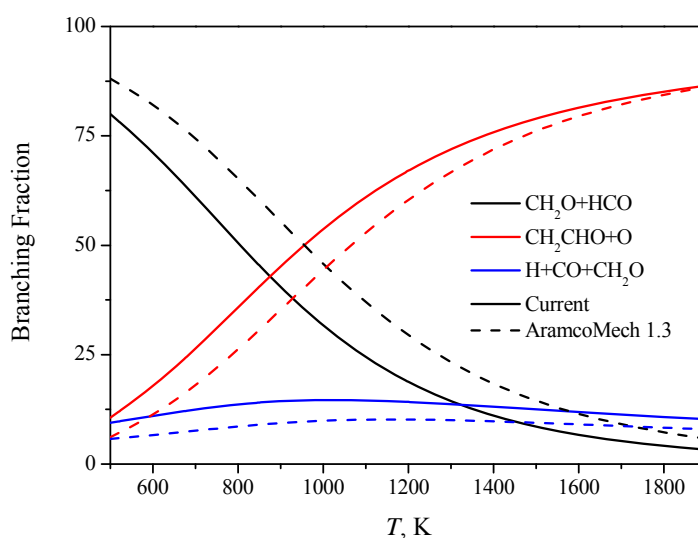


Figure 45: Branching ratio of $\dot{C}_2H_3+O_2 \leftrightarrow$ Products.

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