

Range of experimental conditions used for mechanism validation.

Species	ST	RCM	JSR	FR	FS
H₂	✓	✓	✓	✓	✓
ΔT	952.0 – 1818 K	934.0 – 1040 K	745.0 – 1150 K	880.0 – 1010 K	298.0 K
Δp	1.62 – 270.5 atm	8.0 – 32.0 atm	1.0 – 10.0 atm	0.3 – 15.7 atm	1.0 – 20 atm
$\Delta \phi$	0.1 – 1.0	0.5	0.1 – 2.5	0.4 – 2.0	0.5 – 5.0
H₂/CO	✓	✓	✓	✓	✓
ΔT	909.0 – 129 K	934.0 – 1052 K	840.0 – 1400 K	1040 K	298 – 600 K
Δp	1.05 – 15.5 atm	8.0 – 32.0 atm	1.0 atm	1.0 – 9.7 atm	1.0 – 5.0 atm
$\Delta \phi$	0.5 – 1.0	0.5	0.1 – 2.0	0.5	0.8 – 1.4
CH₃OH	✓	✓	✓	✓	✓
ΔT	909.0 – 2180.0 K	817.0 – 980.0 K	697.2 – 1099.4 K	781.0 – 1043.0 K	298.0 – 423.0 K
Δp	0.99 – 51.71 atm	9.27 – 40.64 atm	10.0 – 10.0 atm	1.0 – 15.0 atm	1.0 – 5.0 atm
$\Delta \phi$	0.38 – 6.0	0.5 – 2.0	0.2 – 0.2	0.42 – 2.59	0.6 – 1.6
CH₄	✓	✓	✓	✓	✓
ΔT	1041.0 – 2538.0 K	869.9 – 1178.19 K	1635.0 – 2400.0 K	1942.0 – 2374.0 K	298.0 K
Δp	0.54 – 260.0 atm	10.0 – 24.0 atm	0.9 – 1.66 atm	0.37 – 1.1 atm	1.0 – 20.0 atm
$\Delta \phi$	0.1 – 6.0	0.3 – 2.0	100.0 – 100.0	0.5 – 4.0	0.6 – 1.6
C₂H₂	✓	✓	×	✓	✓
ΔT	808.6 – 2319.0 K	711.25 – 953.14 K	—	600.0 – 1380.0 K	298.0 K
Δp	0.77 – 31.3 atm	9.04 – 30.37 atm	—	1.0 – 58.82 atm	1.0 – 2.0 atm
$\Delta \phi$	0.06 – 2.0	0.5 – 2.0	—	0.05 – 5.56	0.6 – 2.0
C₂H₄	✓	✓	✓	✓	✓
ΔT	945.2 – 2226.3 K	773.0 – 990.33 K	597.81 – 1300.0 K	850.0 – 1163.0 K	298.0 K
Δp	0.94 – 40.98 atm	19.6 – 41.4 atm	1.0 – 59.22 atm	1.0 – 10.0 atm	1.0 – 5.0 atm
$\Delta \phi$	0.3 – 3.0	0.5 – 2.0	0.5 – 10.0	0.75 – 2.5	0.6 – 1.6
C₂H₅OH	✓	✓	✓	✓	✓
ΔT	778.1 – 1669.8 K	0.0 – 983.12 K	799.0 – 1250.0 K	757.93 – 1400.5 K	298.0 – 428 K
Δp	1.8 – 91.5 atm	0.0 – 50.6 atm	1.0 – 10.0 atm	1.0 – 1.0 atm	1.0 atm
$\Delta \phi$	0.25 – 2.0	0.3 – 2.0	0.25 – 2.0	0.03 – 1.37	0.5 – 1.7
C₂H₆	✓	✓	✓	✓	✓
ΔT	947.3 – 1862.0 K	830.0 – 999.0 K	895.5 – 1215.0 K	598.0 – 1073.0 K	298.0 K
Δp	0.57 – 40.56 atm	19.28 – 81.8 atm	1.0 – 1.0 atm	19.7 – 98.7 atm	1.0 – 10 atm
$\Delta \phi$	0.1 – 2.0	0.5 – 2.0	0.1 – 1.5	0.034 – 1e+30	0.5 – 1.6
CH₃OCH₃	✓	✓	✓	✓	✓
ΔT	666.0 – 1880.9 K	645.0 – 1105.0 K	500.0 – 1205.0 K	580.0 – 1060.0 K	298.0 K
Δp	1.01 – 40.35 atm	9.71 – 22.26 atm	1 – 10 atm	4 – 18 atm	1.0 – 10 atm
$\Delta \phi$	0.5 – 2.0	4.0	0.2 – 2.0	0.68 – 1.52	0.5 – 1.6
C₃H₆	✓	✓	✓	✓	✓
ΔT	999.0 – 1820.0 K	0.0 – 1241.0 K	800.0 – 1426.0 K	800.0 – 1200.0 K	298.0 – 398 K
Δp	0.95 – 47.0 atm	0.0 – 41.62 atm	1.0 – 1.05 atm	1.0 – 15.0 atm	1.0 atm
$\Delta \phi$	0.5 – 2.0	0.5 – 2.0	0.5 – 2.19	0.35 – 1.5	0.5 – 1.6
C₃H₈	✓	✓	✓	✓	✓
ΔT	847.5 – 2615.0 K	714.0 – 909.0 K	674.0 – 1350.0 K	548.0 – 1210.0 K	298.0 K
Δp	0.82 – 41.34 atm	30.0 – 50.0 atm	1.0 – 10.0 atm	1.0 – 98.7 atm	1.0 – 5.0 atm
$\Delta \phi$	0.125 – 2.0	1.0	0.4 – 1.5	0.02 – 4.0	0.5 – 1.6
C₃H₄-a	✓	×	✓	×	×
ΔT	1175.0 – 1896.0 K	—	801.6 – 1261.0 K	—	—
Δp	1.81 – 5.29 atm	—	1.0 – 10.0 atm	—	—
$\Delta \phi$	0.5 – 2.0	—	0.2 – 2.0	—	—
C₃H₄-p	✓	✓	✓	✓	✓
ΔT	1131.0 – 2037.0 K	714.0 – 910.0 K	796.0 – 1265.0 K	1170 K	298.0 – 373 K
Δp	1.8 – 5.26 atm	10.0 – 30.0 atm	1.0 – 10.0 atm	1.0 atm	1.0 – 3.0 atm
$\Delta \phi$	0.5 – 2.0	0.5 – 2.0	0.2 – 2.0	0.7	0.5 – 1.6

C₄H₆	✓	×	×	×	✓
ΔT	954.0 – 1781.7 K	—	—	—	298.0 K
Δp	0.91 – 42.05 atm	—	—	—	1.0 atm
$\Delta \varphi$	0.3 – 2.0	—	—	—	0.5 – 1.6
C₄H₈₋₁	✓	×	×	×	✓
ΔT	899.3 – 1834.5 K	—	—	—	298.0 K
Δp	1.19 – 53.14 atm	—	—	—	1.0 atm
$\Delta \varphi$	0.5 – 2.0	—	—	—	0.5 – 1.6
C₄H₁₀	✓	×	×	×	✓
ΔT	1000.0 – 1430.7 K	—	—	—	298.0 K
Δp	1.0 – 45.05 atm	—	—	—	1.0 atm
$\Delta \varphi$	0.3 – 2.0	—	—	—	0.5 – 1.6
iC₄H₈	✓	✓	×	×	✓
ΔT	987.3 – 1436.5 K	712.0 – 976.0 K	—	—	298.0 – 398 K
Δp	10.0 – 50.0 atm	10.4 – 50.4 atm	—	—	1.0 atm
$\Delta \varphi$	0.3 – 2.0	0.3 – 1.0	—	—	0.5 – 1.6
CH₄/C₂H₄	✓	✓	×	×	×
ΔT	989.5 – 2081.9 K	845.0 – 1105.0 K	—	—	—
Δp	0.89 – 41.04 atm	19.71 – 40.44 atm	—	—	—
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	—	—	—
CH₄/C₂H₆	✓	✓	×	×	✓
ΔT	911.0 – 1700.0 K	909.23 – 966.66 K	—	—	298.0 K
Δp	1.28 – 39.0 atm	39.65 – 40.36 atm	—	—	1.0 – 10.0 atm
$\Delta \varphi$	0.5 – 2.0	1.0 – 1.0	—	—	0.5 – 1.6
C₂H₄/C₂H₆	✓	✓	×	×	×
ΔT	996.0 – 1930.4 K	892.0 – 1041.0 K	—	—	—
Δp	0.9 – 40.57 atm	19.66 – 41.14 atm	—	—	—
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	—	—	—
C₂H₄/C₃H₈	✓	✓	×	×	×
ΔT	910.9 – 2044.5 K	804.0 – 1034.0 K	—	—	—
Δp	0.87 – 40.14 atm	19.5 – 41.22 atm	—	—	—
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	—	—	—
C₂H₆/C₃H₈	✓	✓	×	×	×
ΔT	958.3 – 1998.7 K	836.0 – 1048.0 K	—	—	—
Δp	0.91 – 41.06 atm	19.47 – 137 atm	—	—	—
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	—	—	—
<i>n</i>-C₅H₁₂	✓	✓	✓	×	×
ΔT	770.9 – 1561.5 K	645.0 – 1000.0 K	500.0 – 1100.0 K	—	—
Δp	1.5 – 25.0 atm	10 – 20 atm	1.0 – 10 atm	—	—
$\Delta \varphi$	0.25 – 2.0	0.3 – 2.0	0.25 – 4.0	—	—
<i>i</i>-C₅H₁₂	✓	✓	×	×	×
ΔT	1000 – 1388.5 K	704.0 – 1000.0 K	—	—	—
Δp	10.5 – 25.0 atm	10 – 20 atm	—	—	—
$\Delta \varphi$	0.3 – 2.0	0.3 – 1.0	—	—	—
<i>neo</i>-C₅H₁₂	✓	✓	×	×	×
ΔT	770.9 – 1428.5 K	645.0 – 780.0 K	—	—	—
Δp	10 – 20 atm	10 – 20 atm	—	—	—
$\Delta \varphi$	0.5 – 2.0	0.3 – 2.0	—	—	—
C₅H₁₀₋₁	✓	✓	✓	×	✓

ΔT	900 – 2000 K	600.0 – 900.0 K	750.0 – 1020.0 K	—	353 K
Δp	1 – 30 atm	15 – 30 atm	1.0 atm	—	1.0 – 2.0 atm
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	1.0	—	0.4 – 2.2
C₅H₁₀-2	✓	✓	✓	×	✓
ΔT	900 – 2000 K	600.0 – 900.0 K	750.0 – 1020.0 K	—	353 K
Δp	1 – 30 atm	15 – 30 atm	1.0 atm	—	1.0 – 2.0 atm
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	1.0	—	0.4 – 2.2
C₆H₁₂-1	✓	✓	✓	×	✓
ΔT	750 – 2000 K	600.0 – 1000.0 K	800.0 – 1260.0 K	—	373 K
Δp	2 – 30 atm	15 – 30 atm	1.0 – 10 atm	—	1.0 atm
$\Delta \varphi$	0.5 – 2.0	0.5 – 2.0	0.5 – 4.0	—	0.7 – 1.5
<i>n</i>-C₆H₁₄	✓	✓	✓	×	✓
ΔT	800.0 – 1430.5 K	625.0 – 800.0 K	500.0 – 1100.0 K	—	298.0 – 600 K
Δp	15 – 32.0 atm	15 – 32.0 atm	1.0 – 10 atm	—	1.0 atm
$\Delta \varphi$	1.0 – 2.0	1.0 – 2.0	0.5 – 2.0	—	0.6 – 1.6
<i>n</i>-C₇H₁₆	✓	✓	✓	×	✓
ΔT	800.9 – 1250.5 K	590.0 – 800.0 K	500.0 – 1100.0 K	—	298.0 – 600 K
Δp	13.5 – 55.0 atm	13.5 – 55 atm	1.0 – 10 atm	—	1.0 – 10.0 atm
$\Delta \varphi$	0.25 – 1.0	0.25 – 1.0	0.25 – 4.0	—	0.6 – 1.6