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# 基于不同燃料 PAH 特性改进的适用于多组分燃料的碳烟模型

庞　斌　　解茂昭　　贾　明*　　刘耀东

(大连理工大学能源与动力工程学院, 海洋能源利用与节能教育部重点实验室, 辽宁 大连 116023)

# Improved Phenomenological Soot Model for Multicomponent Fuel Based on Variations in PAH Characteristics with Fuel Type

**PANG Bin　　XIE Mao-Zhao　　JIA Ming*　　LIU Yao-Dong**

(*Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, School of Energy and Power Engineering, Dalian University of Technology, Dalian 116023, Liaoning Province, P. R. China*)

*Corresponding author. Email: jiaming@dlut.edu.cn; Tel: +86-411-84706302.

## CHEMKIN output file for TRF-PAH model

| Species | | | | |
|---|---|---|---|---|
| C7H16 | O2 | CO2 | H2O | CO |
| H2 | OH | H2O2 | HO2 | H |
| O | CH4 | CH3O | CH2O | HCO |
| CH3 | C2H3 | C2H4 | C2H5 | C3H4 |
| C3H5 | C3H6 | C3H7 | C7H15 | C7H15O2 |
| O2C7H14OOH | C7KET | C5H11CO | C7H14 | C8H18 |
| C8H17 | C8H17O2 | C8H16OOH | C8KET | O2C8H16OOH |
| C6H13CO | C8H16 | CH2OH | CH3OH | C7H14OOH |
| C6H5CH2 | C6H5CHO | C6H5CO | C6H5O | C4H5 |
| C4H3 | C5H5 | C5H4O | C5H4OH | C6H5OH |
| C2H2 | CH2CO | HCCO | C5H11 | CH2 |
| C2H | C4H4 | C3H3 | A1 | A1- |
| A2 | A2-1 | A3 | A3-4 | A4 |
| A1C2H* | A1C2H | A4-1 | C9H8 | C9H7 |
| P2 | P2- | C6H5CH3 | | |

| No. Reactions ($k = AT^n\exp(-E/RT)$) | A | n | E |
|---|---|---|---|
| 1. C6H5CH3=C6H5CH2+H | 2.09E+15 | 0.0 | 87463.4 |
| 2. C6H5CH3=>A1-+CH3 | 8.66E+15 | 0.0 | 97830.4 |
| 3. C6H5CH3+O2=C6H5CH2+HO2 | 1.50E+14 | 0.0 | 41400.0 |
| 4. C6H5CH3+H=A1+CH3 | 1.20E+13 | 0.0 | 5100.0 |
| 5. C6H5CH3+OH=C6H5CH2+H2O | 3.00E+12 | 0.0 | 1700.0 |
| 6. C6H5CH2+O=C6H5CHO+H | 2.11E+14 | 0.0 | 0.0 |
| 7. C6H5CH2+O=A1-+CH2O | 1.19E+14 | 0.0 | 0.0 |
| 8. C6H5CH2+HO2=C6H5CHO+H+OH | 1.50E+14 | 0.0 | 0.0 |
| 9. C6H5CHO+OH=H2O+C6H5CO | 3.44E+09 | 1.2 | -447.0 |
| 10. C6H5CHO+H=H2+C6H5CO | 2.28E+10 | 1.1 | 3279.0 |
| 11. C6H5CO=A1-+CO | 3.00E+12 | 0.0 | 34860.0 |
| 12. C6H5O=C5H5+CO | 3.76E+54 | -12.1 | 72800.0 |
| 13. C6H5O+H=C6H5OH | 2.50E+14 | 0.0 | 0.0 |
| 14. C6H5OH+O2=C6H5O+HO2 | 1.00E+13 | 0.0 | 38000.0 |
| 15. C6H5OH+H=C6H5O+H2 | 1.20E+14 | 0.0 | 12400.0 |
| 16. C6H5OH+O=C6H5O+OH | 1.30E+13 | 0.0 | 2900.0 |
| 17. C6H5OH+OH=C6H5O+H2O | 3.00E+06 | 2.0 | -1310.0 |
| 18. C6H5OH+HO2=C6H5O+H2O2 | 1.00E+12 | 0.0 | 1000.0 |
| 19. C5H5+O=C4H5+CO | 4.20E+13 | -0.2 | 440.0 |
| 20. C5H5+OH=C5H4OH+H | 3.50E+57 | -12.2 | 48350.0 |
| 21. C5H4OH=C5H4O+H | 2.10E+13 | 0.0 | 54000.0 |
| 22. C5H4O=>C2H2+C2H2+CO | 5.70E+32 | -6.8 | 68500.0 |
| Declared duplicate reaction... | | | |
| 23. C5H4O=>C2H2+C2H2+CO | 6.20E+41 | -7.9 | 98700.0 |
| Declared duplicate reaction... | | | |

| | | | |
|---|---|---|---|
| 24. C4H5=C2H2+C2H3 | 1.00E+14 | 0.0 | 43890.0 |
| 25. A1-+O2=C6H5O+O | 5.60E+11 | 0.0 | 6100.0 |
| 26. A1+OH=A1-+H2O | 1.63E+08 | 1.4 | 1451.0 |
| 27. A1+O=A1-+OH | 2.00E+13 | 0.0 | 14700.0 |
| 28. C7H16+O2=C7H15+HO2 | 1.00E+16 | 0.0 | 46000.0 |
| Reverse Arrhenius coefficients: | 1.00E+12 | 0.0 | 0.0 |
| 29. C7H15+O2=C7H15O2 | 3.00E+12 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 2.51E+13 | 0.0 | 27400.0 |
| 30. C7H15O2=C7H14OOH | 1.51E+11 | 0.0 | 19000.0 |
| Reverse Arrhenius coefficients: | 1.00E+11 | 0.0 | 11000.0 |
| 31. C7H14OOH+O2=O2C7H14OOH | 6.16E+10 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 2.51E+13 | 0.0 | 27400.0 |
| 32. O2C7H14OOH=>C7KET+OH | 8.91E+10 | 0.0 | 17000.0 |
| 33. C7KET=>C5H11CO+CH2O+OH | 3.98E+15 | 0.0 | 43000.0 |
| 34. C5H11CO+O2=>C3H7+C2H3+CO+HO2 | 3.16E+13 | 0.0 | 10000.0 |
| 35. C7H16+OH=>C7H15+H2O | 5.00E+13 | 0.0 | 3000.0 |
| 36. C7H15+O2=C7H14+HO2 | 3.16E+11 | 0.0 | 6000.0 |
| Reverse Arrhenius coefficients: | 3.16E+11 | 0.0 | 19500.0 |
| 37. C7H14+O2=>C3H6+C2H5+CH2O+HCO | 3.16E+13 | 0.0 | 10000.0 |
| 38. C7H16+HO2=>C7H15+H2O2 | 1.00E+13 | 0.0 | 16950.0 |
| 39. C7H15=>C3H6+C2H5+C2H4 | 6.50E+12 | 0.0 | 28810.0 |
| 40. C8H18+O2=C8H17+HO2 | 3.00E+16 | 0.0 | 46000.0 |
| Reverse Arrhenius coefficients: | 1.00E+12 | 0.0 | 0.0 |
| 41. C8H17+O2=C8H17O2 | 1.00E+12 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 2.51E+13 | 0.0 | 27400.0 |
| 42. C8H17O2=C8H16OOH | 1.51E+11 | 0.0 | 21800.0 |
| Reverse Arrhenius coefficients: | 1.00E+11 | 0.0 | 11000.0 |
| 43. C8H16OOH+O2=O2C8H16OOH | 1.16E+11 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 2.51E+13 | 0.0 | 27400.0 |
| 44. O2C8H16OOH=>C8KET+OH | 8.91E+10 | 0.0 | 17000.0 |
| 45. C8KET=>C6H13CO+CH2O+OH | 3.98E+15 | 0.0 | 43000.0 |
| 46. C6H13CO+O2=>C3H7+C3H5+CO+HO2 | 3.16E+13 | 0.0 | 10000.0 |
| 47. C8H18+OH=>C8H17+H2O | 6.00E+14 | 0.0 | 3000.0 |
| 48. C8H17+O2=C8H16+HO2 | 4.16E+11 | 0.0 | 6000.0 |
| Reverse Arrhenius coefficients: | 3.16E+11 | 0.0 | 19500.0 |
| 49. C8H16+O2=>C3H7+C3H6+CH2O+HCO | 3.16E+13 | 0.0 | 10000.0 |
| 50. C8H18+HO2=>C8H17+H2O2 | 1.00E+13 | 0.0 | 16950.0 |
| 51. C8H17=>C3H7+C3H6+C2H4 | 4.12E+17 | -1.3 | 29700.0 |
| 52. C3H7=C2H4+CH3 | 9.60E+13 | 0.0 | 30950.0 |
| 53. C3H7=C3H6+H | 1.25E+14 | 0.0 | 36900.0 |
| 54. C3H6=C2H3+CH3 | 3.15E+15 | 0.0 | 85500.0 |
| 55. C3H6+CH3=C3H5+CH4 | 9.00E+12 | 0.0 | 8480.0 |
| 56. C3H5+O2=C3H4+HO2 | 6.00E+11 | 0.0 | 10000.0 |
| 57. C3H4+OH=C2H3+CH2O | 1.00E+12 | 0.0 | 0.0 |

| | | | |
|---|---|---|---|
| 58. C3H4+OH=C2H4+HCO | 1.00E+12 | 0.0 | 0.0 |
| 59. C2H5+O2=C2H4+HO2 | 2.00E+10 | 0.0 | -2200.0 |
| 60. C2H4+OH=CH2O+CH3 | 6.00E+13 | 0.0 | 960.0 |
| 61. C2H4+OH=C2H3+H2O | 8.02E+13 | 0.0 | 5955.0 |
| 62. C2H3+O2=CH2O+HCO | 4.00E+12 | 0.0 | -250.0 |
| 63. C2H3+HCO=C2H4+CO | 6.03E+13 | 0.0 | 0.0 |
| 64. C3H5=C2H2+CH3 | 2.40E+48 | -9.9 | 82080.0 |
| Reverse Arrhenius coefficients: | 2.61E+46 | -9.8 | 36950.0 |
| 65. C2H4(+M)=C2H2+H2(+M) | 1.80E+13 | 0.0 | 76000.0 |
| Low pressure limit: 0.15000E+16 | 0.00000E+00 | 0.55440E+05 | |
| 66. C2H3+O2=C2H2+HO2 | 2.12E-06 | 6.0 | 9484.0 |
| Reverse Arrhenius coefficients: | 1.11E-07 | 6.3 | 17570.0 |
| 67. C2H3+H=C2H2+H2 | 2.00E+13 | 0.0 | 2500.0 |
| Reverse Arrhenius coefficients: | 1.33E+13 | 0.0 | 68080.0 |
| 68. C2H2+H(+M)=C2H3(+M) | 3.11E+11 | 0.6 | 2589.0 |
| Low pressure limit: 0.22540E+41 | -0.72690E+01 | 0.65770E+04 | |
| TROE centering: 0.10000E+01 | 0.10000E-14 | 0.67500E+03 | 0.10000E+16 |
| H2 | Enhanced by 2.000E+00 | | |
| H2O | Enhanced by 5.000E+00 | | |
| CO | Enhanced by 2.000E+00 | | |
| CO2 | Enhanced by 3.000E+00 | | |
| 69. C2H2+O2=HCCO+OH | 2.00E+08 | 1.5 | 30100.0 |
| Reverse Arrhenius coefficients: | 2.23E+05 | 1.5 | 25400.0 |
| 70. C2H2+O=HCCO+H | 1.43E+07 | 2.0 | 1900.0 |
| Reverse Arrhenius coefficients: | 2.02E+05 | 2.0 | 13310.0 |
| 71. C2H2+OH=CH2CO+H | 2.19E-04 | 4.5 | -1000.0 |
| Reverse Arrhenius coefficients: | 2.16E-03 | 4.5 | 19660.0 |
| 72. CH2CO+H=CH3+CO | 1.10E+13 | 0.0 | 3400.0 |
| Reverse Arrhenius coefficients: | 2.40E+12 | 0.0 | 40200.0 |
| 73. CH2CO+O=HCCO+OH | 1.00E+13 | 0.0 | 8000.0 |
| Reverse Arrhenius coefficients: | 1.43E+10 | 0.0 | -1255.0 |
| 74. CH2CO+OH=HCCO+H2O | 1.00E+13 | 0.0 | 2000.0 |
| Reverse Arrhenius coefficients: | 1.41E+11 | 0.0 | 9995.0 |
| 75. CH2CO+H=HCCO+H2 | 2.00E+14 | 0.0 | 8000.0 |
| Reverse Arrhenius coefficients: | 6.52E+11 | 0.0 | 840.0 |
| 76. HCCO+OH=HCO+HCO | 1.00E+13 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 2.41E+14 | 0.0 | 40360.0 |
| 77. HCCO+O=H+CO+CO | 8.00E+13 | 0.0 | 0.0 |
| Reverse Arrhenius coefficients: | 0.00E+00 | 0.0 | 0.0 |
| 78. HCCO+O2=CO2+HCO | 2.40E+11 | 0.0 | -854.0 |
| Reverse Arrhenius coefficients: | 1.47E+14 | 0.0 | 133600.0 |
| 79. H+O2=O+OH | 3.55E+15 | -0.4 | 16599.0 |
| 80. O+H2=H+OH | 5.08E+04 | 2.7 | 6290.0 |
| 81. H2+OH=H2O+H | 2.16E+08 | 1.5 | 3430.0 |

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|---|---|---|---|---|
| 82. O+H2O=OH+OH | | 2.97E+06 | 2.0 | 13400.0 |
| 83. H2+M=H+H+M | | 4.58E+19 | -1.4 | 104380.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 84. O+O+M=O2+M | | 6.16E+15 | -0.5 | 0.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 85. O+H+M=OH+M | | 4.71E+18 | -1.0 | 0.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 86. H+OH+M=H2O+M | | 3.80E+22 | -2.0 | 0.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 87. H+O2(+M)=HO2(+M) | | 1.48E+12 | 0.6 | 0.0 |
| Low pressure limit: | 0.63660E+21 | -0.17200E+01 | 0.52480E+03 | |
| TROE centering: | 0.80000E+00 | 0.10000E-29 | 0.10000E+31 | |
| H2 | Enhanced by 2.000E+00 | | | |
| H2O | Enhanced by 1.100E+01 | | | |
| O2 | Enhanced by 7.800E-01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 88. HO2+H=H2+O2 | | 1.66E+13 | 0.0 | 823.0 |
| 89. HO2+H=OH+OH | | 7.08E+13 | 0.0 | 295.0 |
| 90. HO2+O=O2+OH | | 3.25E+13 | 0.0 | 0.0 |
| 91. HO2+OH=H2O+O2 | | 2.89E+13 | 0.0 | -497.0 |
| 92. HO2+HO2=H2O2+O2 | | 4.20E+14 | 0.0 | 11982.0 |
| Declared duplicate reaction... | | | | |
| 93. HO2+HO2=H2O2+O2 | | 1.30E+11 | 0.0 | -1629.3 |
| Declared duplicate reaction... | | | | |
| 94. H2O2(+M)=OH+OH(+M) | | 2.95E+14 | 0.0 | 48430.0 |
| Low pressure limit: | 0.12020E+18 | 0.00000E+00 | 0.45500E+05 | |
| TROE centering: | 0.50000E+00 | 0.10000E-29 | 0.10000E+31 | |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |

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|---|---|---|---|---|
| 95. H2O2+H=H2O+OH | | 2.41E+13 | 0.0 | 3970.0 |
| 96. H2O2+H=HO2+H2 | | 4.82E+13 | 0.0 | 7950.0 |
| 97. H2O2+O=OH+HO2 | | 9.55E+06 | 2.0 | 3970.0 |
| 98. H2O2+OH=HO2+H2O | | 1.00E+12 | 0.0 | 0.0 |
| Declared duplicate reaction... | | | | |
| 99. H2O2+OH=HO2+H2O | | 5.80E+14 | 0.0 | 9557.0 |
| Declared duplicate reaction... | | | | |
| 100. CO+O(+M)=CO2(+M) | | 1.80E+10 | 0.0 | 2384.0 |
| Low pressure limit: | 0.15500E+25 | -0.27900E+01 | 0.41910E+04 | |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 101. CO+O2=CO2+O | | 2.53E+12 | 0.0 | 47700.0 |
| 102. CO+HO2=CO2+OH | | 3.01E+13 | 0.0 | 23000.0 |
| 103. CO+OH=CO2+H | | 2.23E+05 | 1.9 | -1158.7 |
| 104. HCO+M=H+CO+M | | 4.75E+11 | 0.7 | 14874.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 6.000E+00 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 105. HCO+O2=CO+HO2 | | 7.58E+12 | 0.0 | 410.0 |
| 106. HCO+H=CO+H2 | | 7.23E+13 | 0.0 | 0.0 |
| 107. HCO+O=CO+OH | | 3.02E+13 | 0.0 | 0.0 |
| 108. HCO+OH=CO+H2O | | 3.02E+13 | 0.0 | 0.0 |
| 109. HCO+O=CO2+H | | 3.00E+13 | 0.0 | 0.0 |
| 110. HCO+HO2=CO2+OH+H | | 3.00E+13 | 0.0 | 0.0 |
| 111. HCO+CH3=CO+CH4 | | 1.20E+14 | 0.0 | 0.0 |
| 112. HCO+HCO=H2+CO+CO | | 3.00E+12 | 0.0 | 0.0 |
| 113. HCO+HCO=CH2O+CO | | 3.00E+13 | 0.0 | 0.0 |
| 114. CH2O+M=HCO+H+M | | 3.30E+39 | -6.3 | 99900.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 115. CH2O+M=CO+H2+M | | 3.10E+45 | -8.0 | 97510.0 |
| H2 | Enhanced by 2.500E+00 | | | |
| H2O | Enhanced by 1.200E+01 | | | |
| CO | Enhanced by 1.900E+00 | | | |
| CO2 | Enhanced by 3.800E+00 | | | |
| 116. CH2O+H=HCO+H2 | | 5.74E+07 | 1.9 | 2748.6 |
| 117. CH2O+O=HCO+OH | | 1.81E+13 | 0.0 | 3080.0 |
| 118. CH2O+OH=HCO+H2O | | 3.43E+09 | 1.2 | -447.0 |
| 119. CH2O+O2=HCO+HO2 | | 1.23E+06 | 3.0 | 52000.0 |

| | | | |
|---|---|---|---|
| 120. CH2O+HO2=HCO+H2O2 | 4.11E+04 | 2.5 | 10210.0 |
| 121. CH2O+CH3=HCO+CH4 | 3.64E-06 | 5.4 | 998.0 |
| 122. CH3+O=CH2O+H | 8.43E+13 | 0.0 | 0.0 |
| 123. CH3+O2=CH3O+O | 1.99E+18 | -1.6 | 29230.0 |
| 124. CH3+O2=CH2O+OH | 3.74E+11 | 0.0 | 14640.0 |
| 125. CH3+HO2=CH3O+OH | 2.41E+10 | 0.8 | -2325.0 |
| 126. CH3+H(+M)=CH4(+M) | 1.27E+16 | -0.6 | 383.0 |
| Low pressure limit: 0.24770E+34 | -0.47600E+01 | 0.24400E+04 | |
| TROE centering: 0.78300E+00 | 0.74000E+02 | 0.29410E+04 | 0.69640E+04 |
| H2 | Enhanced by 2.000E+00 | | |
| H2O | Enhanced by 6.000E+00 | | |
| CH4 | Enhanced by 2.000E+00 | | |
| CO | Enhanced by 1.500E+00 | | |
| CO2 | Enhanced by 2.000E+00 | | |
| 127. CH4+H=CH3+H2 | 5.47E+07 | 2.0 | 11210.0 |
| 128. CH4+O=CH3+OH | 3.15E+12 | 0.5 | 10290.0 |
| 129. CH4+OH=CH3+H2O | 5.72E+06 | 2.0 | 2639.0 |
| 130. CH3+HO2=CH4+O2 | 3.16E+12 | 0.0 | 0.0 |
| 131. CH4+HO2=CH3+H2O2 | 1.81E+11 | 0.0 | 18580.0 |
| 132. CH2OH+M=CH2O+H+M | 1.00E+14 | 0.0 | 25100.0 |
| 133. CH2OH+H=CH2O+H2 | 6.00E+12 | 0.0 | 0.0 |
| 134. CH2OH+H=CH3+OH | 9.64E+13 | 0.0 | 0.0 |
| 135. CH2OH+O=CH2O+OH | 4.20E+13 | 0.0 | 0.0 |
| 136. CH2OH+OH=CH2O+H2O | 2.40E+13 | 0.0 | 0.0 |
| 137. CH2OH+O2=CH2O+HO2 | 2.41E+14 | 0.0 | 5017.0 |
| Declared duplicate reaction... | | | |
| 138. CH2OH+O2=CH2O+HO2 | 1.51E+15 | -1.0 | 0.0 |
| Declared duplicate reaction... | | | |
| 139. CH2OH+HO2=CH2O+H2O2 | 1.20E+13 | 0.0 | 0.0 |
| 140. CH2OH+HCO=CH3OH+CO | 1.00E+13 | 0.0 | 0.0 |
| 141. CH2OH+HCO=CH2O+CH2O | 1.50E+13 | 0.0 | 0.0 |
| 142. 2CH2OH=CH3OH+CH2O | 3.00E+12 | 0.0 | 0.0 |
| 143. CH2OH+CH3O=CH3OH+CH2O | 2.40E+13 | 0.0 | 0.0 |
| 144. CH3O+M=CH2O+H+M | 8.30E+17 | -1.2 | 15500.0 |
| 145. CH3O+H=CH3+OH | 3.20E+13 | 0.0 | 0.0 |
| 146. CH3O+O=CH2O+OH | 6.00E+12 | 0.0 | 0.0 |
| 147. CH3O+OH=CH2O+H2O | 1.80E+13 | 0.0 | 0.0 |
| 148. CH3O+O2=CH2O+HO2 | 9.03E+13 | 0.0 | 11980.0 |
| Declared duplicate reaction... | | | |
| 149. CH3O+O2=CH2O+HO2 | 2.20E+10 | 0.0 | 1748.0 |
| Declared duplicate reaction... | | | |
| 150. CH3O+HO2=CH2O+H2O2 | 3.00E+11 | 0.0 | 0.0 |
| 151. CH3O+CO=CH3+CO2 | 1.60E+13 | 0.0 | 11800.0 |
| 152. CH3O+HCO=CH3OH+CO | 9.00E+13 | 0.0 | 0.0 |

153. 2CH3O=CH3OH+CH2O 6.00E+13 0.0 0.0
154. OH+CH3(+M)<=>CH3OH(+M) 2.79E+18 -1.4 1330.0
Low pressure limit: 0.40000E+37 -0.59200E+01 0.31400E+04
TROE centering: 0.41200E+00 0.19500E+03 0.59000E+04 0.63940E+04
H2 Enhanced by 2.000E+00
H2O Enhanced by 6.000E+00
CH4 Enhanced by 2.000E+00
CO Enhanced by 1.500E+00
CO2 Enhanced by 2.000E+00
155. H+CH2OH(+M)<=>CH3OH(+M) 1.06E+12 0.5 86.0
Low pressure limit: 0.43600E+32 -0.46500E+01 0.50800E+04
TROE centering: 0.60000E+00 0.10000E+03 0.90000E+05 0.10000E+05
H2 Enhanced by 2.000E+00
H2O Enhanced by 6.000E+00
CH4 Enhanced by 2.000E+00
CO Enhanced by 1.500E+00
CO2 Enhanced by 2.000E+00
156. H+CH3O(+M)<=>CH3OH(+M) 2.43E+12 0.5 50.0
Low pressure limit: 0.46600E+42 -0.74400E+01 0.14080E+05
TROE centering: 0.70000E+00 0.10000E+03 0.90000E+05 0.10000E+05
H2 Enhanced by 2.000E+00
H2O Enhanced by 6.000E+00
CH4 Enhanced by 2.000E+00
CO Enhanced by 1.500E+00
CO2 Enhanced by 2.000E+00
157. CH3OH+H=CH2OH+H2 3.20E+13 0.0 6095.0
158. CH3OH+H=CH3O+H2 8.00E+12 0.0 6095.0
159. CH3OH+O=CH2OH+OH 3.88E+05 2.5 3080.0
160. CH3OH+OH=CH3O+H2O 1.00E+06 2.1 496.7
161. CH3OH+OH=CH2OH+H2O 7.10E+06 1.8 -596.0
162. CH3OH+O2=CH2OH+HO2 2.05E+13 0.0 44900.0
163. CH3OH+HCO=CH2OH+CH2O 9.64E+03 2.9 13110.0
164. CH3OH+HO2=CH2OH+H2O2 3.98E+13 0.0 19400.0
165. CH3OH+CH3=CH2OH+CH4 3.19E+01 3.2 7172.0
166. CH3O+CH3OH=CH3OH+CH2OH 3.00E+11 0.0 4060.0
167. C8H18=C5H11+C3H7 2.00E+12 0.0 77990.4
168. C7H16=C7H15+H 3.97E+10 -0.9 103200.0
169. C6H5CH2=C5H5+C2H2 1.00E+06 0.0 34879.4
170. C6H5CH2=C4H4+C3H3 8.00E+12 0.0 83376.1
171. CH2+CH2=C2H2+H2 1.20E+13 0.0 800.0
172. CH2+CH2=C2H2+H+H 1.20E+14 0.0 800.0
173. C2H2+O=CH2+CO 4.05E+05 2.0 1900.0
174. C2H2+O=C2H+OH 4.60E+19 -1.4 28950.0

| | | | |
|---|---|---|---|
| Reverse Arrhenius coefficients: | 3.02E+15 | -0.6 | -1782.0 |
| 175. CH2+C2H2=C3H3+H | 2.40E+13 | 0.0 | 6620.0 |
| 176. C2H2+CH3=C3H4+H | 2.72E+18 | -2.0 | 20200.0 |
| 177. C3H4+H=C3H3+H2 | 1.15E+08 | 1.9 | 7530.0 |
| 178. C3H3+OH=C2H3+HCO | 2.00E+13 | 0.0 | 0.0 |
| 179. C2H2+C2H3=C4H4+H | 4.90E+16 | -1.1 | 11800.0 |
| 180. C3H3+C2H2=C5H5 | 6.35E+10 | 0.0 | 9995.2 |
| 181. C3H3+O2=CH2CO+HCO | 3.00E+10 | 0.0 | 2878.0 |
| 182. C3H3+C3H3=A1 | 8.56E+19 | -2.5 | 1692.0 |
| 183. C3H4+C3H3=A1+H | 4.40E+08 | 0.0 | 2000.0 |
| 184. A1=A1-+H | 1.29E+62 | -12.5 | 148085.6 |
| 185. A1+H=A1-+H2 | 2.50E+14 | 0.0 | 16000.0 |
| 186. A1+CH3=>A1-+CH4 | 4.42E+01 | 3.9 | 11463.0 |
| 187. A1+C3H3=C9H8+H | 6.26E+09 | 2.6 | 56500.0 |
| 188. A1+O=C6H5O+H | 2.20E+13 | 0.0 | 4530.0 |
| 189. A1+OH=C6H5OH+H | 1.30E+13 | 0.0 | 10600.0 |
| 190. A1-+C4H4=A2+H | 2.50E+29 | -4.4 | 26400.0 |
| 191. 2C5H5=A2+2H | 6.10E+10 | 0.0 | 4888.3 |
| 192. A1-+C2H2=A1C2H+H | 2.50E+29 | -4.4 | 26400.0 |
| 193. A1C2H+H=A1C2H*+H2 | 2.50E+14 | 0.0 | 16000.0 |
| 194. A1C2H+OH=A1C2H*+H2O | 1.60E+08 | 1.4 | 1450.0 |
| 195. A2-1+C4H4=A3+H | 2.50E+26 | -4.4 | 26400.0 |
| 196. A1+A1-=P2+H | 1.10E+23 | -2.9 | 15890.0 |
| 197. P2+H=P2-+H2 | 2.50E+14 | 0.0 | 16000.0 |
| 198. P2-+C2H2=A3+H | 4.60E+06 | 2.0 | 7300.0 |
| 199. A1C2H*+A1=A3+H | 1.10E+24 | -2.9 | 15890.0 |
| 200. A1-+A1C2H=A3+H | 1.10E+24 | -2.9 | 15890.0 |
| 201. A3-4+C2H2=A4+H | 1.40E+26 | -3.4 | 17800.0 |
| 202. C9H8=C9H7+H | 1.73E+68 | -15.2 | 116371.9 |
| 203. C9H7+C9H7=>A4+C2H2+H2 | 6.39E+29 | -4.0 | 35205.5 |
| 204. C9H7+C5H5=>A3+2H | 6.39E+29 | -4.0 | 35205.5 |
| 205. A2+H=>A2-1+H2 | 2.20E+07 | 1.9 | 9829.5 |
| 206. A3+H=>A3-4+H2 | 3.00E+08 | 1.9 | 9829.5 |
| 207. A4+CH3=>A4-1+CH4 | 2.40E+00 | 3.9 | 11771.0 |