Supplemental Material for

**Experimental and kinetic modeling study of ignition characteristics of RP-3 kerosene over low-to-high temperature ranges in a heated rapid compression machine and a heated shock tube**

Table S3 Modification of the mechanism

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| --- | --- | --- |
| Reactions | Modification | Source |
| NC12H26+O2<=>NC12H25+HO2 7.00E+12 0.0 27800.0  REV / 1.00E+12 0.0 0.0 / | Added | [1] |
| NC12H26+OH<=>NC12H25+H2O 5.00E+07 1.9 58.5  REV / 6.15E+08 1.9 21910.0 / | Added | [1] |
| NC12H26+H=>NC12H25+H2 1.00E+08 2.0 2500.0 | Added | [1] |
| NC12H25+O2<=> NC12H25-OO 3.00E+12 0.0 0.0  REV / 2.51E+13 0.0 27400.0 / | Added | [1] |
| NC12H25-OO <=> NC12-QOOH 1.51E+11 0.0 19000.0  REV / 1.00E+11 0.0 11000.0 / | Added | [1] |
| NC12-QOOH +O2<=> NC12-OOQOOH 5.56E+10 0.0 0.0  REV / 2.51E+13 0.0 27400.0 / | Added | [1] |
| NC12-OOQOOH<=> NC12-OQOOH+OH 6.0000e+12 0.000 26000.00 | Added | [1] |
| NC12-OQOOH =>CH2O+C5H11CO+OH+C3H6+C2H4 1.98E+15 0.0 43000.0 | Added | [1] |
| C5H11CO+O2=>NC3H7+C2H3+CO+HO2 3.16E+13 0.0 10000.0 | Added | [1] |
| NC12H25+O2=C12H24+HO2 3.16E+11 0.0 6000.0  REV / 3.16E+11 0.0 19500.0 / | Added | [1] |
| C12H24+O2=>2C3H6 +C2H5+CH2O+HCO+C2H4 3.16E+13 0.0 10000.0 | Added | [1] |
| NC12H25=>2C3H6+C2H5+2C2H4 3.50E+12 0.0 28810.0 | Added | [1] |
| NC12H26=>0.5C2H5+0.5NC3H7+0.5NC7H15+0.5NC12H25 2.2500e+17 0.000 81000.00 | Deleted | [2] |
| NC12H26=>0.5NC4H9P+0.5NC5H11+0.9NC7H15+0.1NC12H25 2.2500e+17 0.000 81000.00 | Deleted | [2] |
| O2+NC12H26=>HO2+NC12H25 3.0000e+14 0.000 45000.00 | Deleted | [2] |
| NC12H26+OH=>H2O+NC12H25 8.7870e+06 2.000 -2259.83 | Deleted | [2] |
| NC12H26+CH2OH=>CH3OH+NC12H25 6.2210e+05 2.000 10472.57 | Deleted | [2] |
| NC12H26+H=>H2+NC12H25 5.2950e+07 2.000 3950.57 | Deleted | [2] |
| NC12H26+CH3=>CH4+NC12H25 8.5870e+05 2.000 4871.29 | Deleted | [2] |
| NC12H26+CH3CO3=>CH3CO3H+NC12H25 7.4790e+05 2.000 6260.57 | Deleted | [2] |
| NC12H26+CH3OO=>CH3OOH+NC12H25 1.6740e+06 2.000 12360.44 | Deleted | [2] |
| NC12H26+CH3CO=>CH3CHO+NC12H25 2.9770e+06 2.000 14065.90 | Deleted | [2] |
| NC12H26+HCO=>CH2O+NC12H25 2.7790e+06 2.000 12360.44 | Deleted | [2] |
| NC12H26+CH2CHO=>CH3CHO+NC12H25 5.0560e+05 2.000 11415.50 | Deleted | [2] |
| NC12H26+C3H3=>AC3H4+NC12H25 5.9410e+05 2.000 14730.58 | Deleted | [2] |
| NC12H26+HCCO=>CH2CO+NC12H25 9.4150e+05 2.000 5333.37 | Deleted | [2] |
| NC12H26+CHCHCH3=>C3H6+NC12H25 5.9410e+05 2.000 4594.58 | Deleted | [2] |
| NC12H26+C2H3=>C2H4+NC12H25 1.4920e+06 2.000 4871.29 | Deleted | [2] |
| NC12H26+C4H5=>C4H6+NC12H25 5.9410e+05 2.000 4594.58 | Deleted | [2] |
| NC12H26+SC4H7=>NC4H8+NC12H25 7.4790e+05 2.000 15253.34 | Deleted | [2] |
| NC12H26+CH2C3H5=>NC4H8+NC12H25 2.9770e+05 2.000 6725.57 | Deleted | [2] |
| NC12H26+NC3H7=>C3H8+NC12H25 2.9770e+05 2.000 6632.50 | Deleted | [2] |
| NC12H26+C6H5O=>C6H5OH+NC12H25 5.9410e+05 2.000 12549.65 | Deleted | [2] |
| NC12H26+C2H5=>C2H6+NC12H25 5.0560e+05 2.000 7658.07 | Deleted | [2] |
| NC12H26+CH3O=>CH3OH+NC12H25 9.4150e+05 2.000 1583.56 | Deleted | [2] |
| NC12H26+O=>OH+NC12H25 2.9770e+07 2.000 2579.54 | Deleted | [2] |
| NC12H26+HO2=>H2O2+NC12H25 1.1850e+06 2.000 11887.73 | Deleted | [2] |
| NC12H26+CH2CHCH2=>C3H6+NC12H25 5.2950e+05 2.000 15253.34 | Deleted | [2] |
| NC12H26+IC3H7=>C3H8+NC12H25 2.9770e+05 2.000 8593.61 | Deleted | [2] |
| NC12H26+C4H3=>C4H4+NC12H25 8.9920e+05 2.000 5333.37 | Deleted | [2] |
| NC12H26+IC4H7=>IC4H8+NC12H25 7.4790e+05 2.000 15253.34 | Deleted | [2] |
| NC12H26+CH2CCH3=>C3H6+NC12H25 5.9410e+05 2.000 4594.58 | Deleted | [2] |
| NC12H26+C6H5=>C6H6+NC12H25 2.9770e+05 2.000 -111.23 | Deleted | [2] |
| NC12H26+C2H5OO=>C2H5OOH+NC12H25 1.6740e+06 2.000 12360.44 | Deleted | [2] |
| NC12H26+CH3COCH2=>CH3COCH3+NC12H25 5.0560e+05 2.000 7658.07 | Deleted | [2] |
| NC12H26+C5H7=>C5H8+NC12H25 5.9410e+05 2.000 15205.80 | Deleted | [2] |
| NC12H26+C7H7=>C7H8+NC12H25 5.9410e+05 2.000 14730.58 | Deleted | [2] |
| NC12H26+C6H4CH3=>C7H8+NC12H25 2.9770e+05 2.000 -111.23 | Deleted | [2] |
| NC12H26+RCRESOLO=>CRESOL+NC12H25 5.9410e+05 2.000 12549.65 | Deleted | [2] |
| NC12H26+HCO3=>HCO3H+NC12H25 7.4790e+05 2.000 6260.57 | Deleted | [2] |
| NC12H26+INDENYL=>INDENE+NC12H25 2.9770e+05 2.000 15681.39 | Deleted | [2] |
| NC12H26+C10H7=>C10H8+NC12H25 1.8790e+05 2.000 -111.23 | Deleted | [2] |
| NC12H26+C6H5C2H2=>C6H5C2H3+NC12H25 2.9770e+05 2.000 -111.23 | Deleted | [2] |
| NC12H26+NC7H13=>NC7H14+NC12H25 5.9410e+05 2.000 10943.77 | Deleted | [2] |
| NC12H26+NC10H19=>NC10H20+NC12H25 5.9410e+05 2.000 10943.77 | Deleted | [2] |
| O2+NC12H25=>1.2NC10H20+HO2 5.0000e+11 0.000 3500.00 | Deleted | [2] |
| O2+NC12H25=>NC12H25-OO 2.0000e+12 0.000 0.00 | Deleted | [2] |
| NC12H25-OO=>O2+NC12H25 5.0000e+13 0.000 31000.00 | Deleted | [2] |
| NC12H25-OO=>NC12-QOOH 3.0000e+12 0.000 24000.00 | Deleted | [2] |
| NC12-QOOH=>NC12H25-OO 2.0000e+10 0.000 16100.00 | Deleted | [2] |
| HO2+NC12H25-OO=>O2+NC7H15OOH+0.5NC10H20 1.0000e+11 0.000 -2600.00 | Deleted | [2] |
| 2NC12H25-OO =>O2+2CH2O+2C2H4+0.6667NC7H15+1.33330NC10H21 5.0000e+10 0.000 -2600.00 | Deleted | [2] |
| 2NC12H25-OO=>O2+2C2H5CHO+0.6667NC7H15+1.33330NC10H21 2.5000e+10 0.000 -2600.00 | Deleted | [2] |
| HO2+NC12-OOQOOH=>2O2+NC7H15OOH+0.5NC10H20 1.0000e+11 0.000 -2600.00 | Deleted | [2] |
| NC12H25-OO+NC12-OOQOOH =>2O2+2C2H5CHO+0.6667NC7H15+1.33330NC10H21 7.5000e+10 0.000 -2600.00 | Deleted | [2] |
| NC12-QOOH=>NC5H10+NC7H14O+OH 1.5000e+10 0.000 14100.00 | Deleted | [2] |
| NC12-QOOH=>1.2NC10H20+HO2 4.5000e+11 0.000 19000.00 | Deleted | [2] |
| NC12-QOOH =>CH2O+0.35C3H6+0.35NC5H10+0.6NC7H14+0.4NC10H20+OH 6.0000e+11 0.000 22500.00 | Deleted | [2] |
| NC12-QOOH=>0.7C2H4+CH3CHO+0.8NC7H14+0.3NC10H20+OH 7.0000e+11 0.000 22500.00 | Deleted | [2] |
| O2+NC12-QOOH=>NC12-OOQOOH 2.0000e+12 0.000 0.00 | Deleted | [2] |
| NC12-OOQOOH=>O2+NC12-QOOH 2.0000e+14 0.000 29000.00 | Deleted | [2] |
| NC12-OOQOOH=>NC12-OQOOH+OH 6.0000e+12 0.000 26000.00 | Deleted | [2] |
| NC12-OOQOOH=>NC12-OQOOH+OH 6.0000e+12 0.000 26000.00 | Deleted | [2] |
| NC12-OQOOH=>CH2O+0.25NC4H8+0.8NC10H20+OH+CH3CO 1.8500e+14 0.000 39000.00 | Deleted | [2] |
| NC12-OQOOH =>0.84CO+CH3CHO+NC7H14+OH+0.84C2H5+0.16CH3COCH2 3.3000e+14 0.000 39000.00 | Deleted | [2] |
| NC12-OQOOH=>CO+0.5CH2O+0.5C2H5CHO+NC7H14+OH+C2H5 2.52E+14 0.000 39000.00 !SPLIT MAX 6 PROD | Deleted | [2] |
| NC12-OQOOH=>0.5CH2O+0.5C2H5CHO+NC7H14+OH+CH3COCH2 4.8E+13 0.000 39000.00 !SPLIT MAX 6 PROD | Deleted | [2] |

**Figure S1.** validation of the modified model against the existing experimental data in literature [3]







Reference

[1] Y. Chang, M. Jia, Y. Liu, Y. Li, M. Xie, H. Yin, Application of a Decoupling Methodology for Development of Skeletal Oxidation Mechanisms for Heavy n-Alkanes from n-Octane to n-Hexadecane, Energy & Fuels 27 (2013) 3467-3479.

[2] E. Ranzi, A. Frassoldati, A. Stagni, M. Pelucchi, A. Cuoci, T. Faravelli, Reduced Kinetic Schemes of Complex Reaction Systems: Fossil and Biomass-Derived Transportation Fuels, Int. J. Chem. Kinet. 46 (2014) 512-542.

[3] C. Zhang, B. Li, F. Rao, P. Li, X. Li, A shock tube study of the autoignition characteristics of RP-3 jet fuel, Proc. Combust. Inst. 35 (2015) 3151-3158.