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- (1) The Kinetic Nonequilibrium Processes in the Internal Flow and in the Plume of Subsonic and Supersonic Aircrafts
- (2) Summary of Research
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Summary of Research

The research work have been carried out in the following directions:

1. The development of the kinetic models for detailed description of formation of ecological dangerous species under combustion hydrocarbon (hydrogen)+air mixtures.

For the analysis of nonequilibrium kinetic processes under combustion of hydrocarbon (hydrogen)+air mixtures we have developed the kinetic scheme including 562 reversible reactions with participation of 83 components. The coefficients A , m , E_a for calculation of rate constants of reactions ($k(T)=AT^m\exp(E_a/T)$) were taken on the base of recommendation [1-8]. The reactions list for this model and coefficients A , m , E_a are presented in *Table 1*. We have analysed the kinetic processes under combustion of the products of thermal destruction of $n\text{-C}_8\text{H}_{18}$ in air with various values of the equivalence ratio α . In *Table 2* the mixture compositions (in mole fraction) for air+products of $n\text{-C}_8\text{H}_{18}$ destruction with $\alpha=1$; 0.5; 0.25 under $T_0=1000\text{ K}$ and $P_0=1\text{ MPa}$ are presented. The composition of the products of thermal destruction of $n\text{-C}_8\text{H}_{18}$ was taken from experimental investigation [9]. The mixture contains significant proportions of H_2 , CH_4 , C_2H_4 , C_2H_6 , C_3H_8 , $n\text{-C}_4\text{H}_{10}$. So the developed kinetic scheme must certainly describe the induction time and other characteristics of combustion not only for CH_4 or $\text{CH}_2/\text{C}_2\text{H}_2$ as it have been supposed before, but also for H_2 , C_2H_6 , C_3H_8 , and $n\text{-C}_4\text{H}_{10}$. Our scheme admits do it. The results of calculation of gas composition (in mole fraction) and temperature at various moments for the model situation of combustion of the products of destruction $n\text{-C}_8\text{H}_{18}$ +air and CH_4 +air with $\alpha=0.25$, $T_0=1000\text{ K}$, $P_0=1\text{ MPa}$ (we have considered the homogeneous reaction in a closed volume and used a model of nonviscous non-heat-conducting gas) are presented in *Table 3*. These results show that chemical equilibrium for the most of small components such as NO_2 , NO_3 , HNO , HNO_2 , HNO_3 , N_x , H_y , OH , HO_2 and others is realized only at very much time ($t=60\text{ sec}$), and that the modeling of kinetic formation of NO_x , HNO_x , HO_x , N_xH_y , C_xH_x and other species under combustion $n\text{-C}_8\text{H}_{18}$ +air mixtures using the reactions mechanisms for CH_4 +air mixture may lead to significant mistakes.

2. The numerical simulations chemical kinetics of formation of N-, H-, C- containing species in the internal flow of subsonic and supersonic aircraft with hydrocarbon and hydrogen combustion engine.

For the analysis of nonequilibrium chemical processes in the internal flow of gas turbine engine for subsonic aircraft and ramjet engine for hypersonic aircraft we have developed quasi one-dimensional models. The kinetic scheme which was used for calculation of variation component concentrations in the gas engine elements includes 229 reversible chemical reactions with participation of 41 components. We reduced the complete scheme (see *Table 1*) excluding the reactions with participation of C_2 -, C_3 -, C_4 -containing species. The previously analysis have been carried out for internal flow of gas-turbine engine *RB211-524B* for *B-747* aircraft and for ramjet axisymmetric hydrogen combustion engine [10]. The geometrical schemes of these engines presented in Performance Report. For *RB211-524B* engine we have considered two different boundary conditions of gas composition at the exit plane of combustion chamber. The first ones corresponded to equilibrium gas composition under combustion $n\text{-C}_8\text{H}_{18}$ +air mixture with

$\alpha=0.25$ and the second ones were taken from nonequilibrium calculation of combustion of products of destruction $n\text{-C}_8\text{H}_{18}$ +air mixture under $\alpha=0.25$; $T_0=1000\text{ K}$; $P_0=1\text{ MPa}$ for $t=4\cdot 10^{-2}\text{ s}$. The values of temperature T , pressure P and gas composition at the mixture (in mole fraction) in different cross section of the gas-turbine engine *RB211-524B* for flight regime: $H=10.7\text{ km}$, $P_e=23.39\text{ kPa}$, $T_e=218.5\text{ K}$, $M_e=0.8$ are presented in for these different conditions in *Table 4* and *5* correspondingly. The obtained results point out on the significant dependence of the gas composition at the exit nozzle plane from boundary conditions at the exit of combustion chamber and from nonequilibrium chemical processes in the internal flow of engine elements.

3. The development of the models for detailed description of gas-phase chemistry and study nonequilibrium processes in the near field plume of subsonic and supersonic aircraft.

For analysis of chemical and photochemical nonequilibrium processes in the near field plume we have developed quasi one-dimensional (*QID*) and two dimensional (*2D*) model.

The *QID*-model contains the gasdynamic block in which the gasdynamic parameters are calculated taking into account the turbulent mixing of exhaust flow with free stream of atmosphere air containing all gas small components, and the kinetic block in which variation of component concentrations along the plume is calculated using quasi one-dimensional approximation and average values of velocity, density, and temperature.

The developed scheme of chemical processes includes reactions characterized both for the high temperature conditions and for the atmospheric photochemistry and contains 237 chemical and 28 photochemical reactions with participation of 61 components. The chemical reactions and photodissociation reaction list for plume kinetic model are presented in *Tables 6, 7*.

We have simulated the nonequilibrium chemical processes in the plume for subsonic aircraft with gas-turbine hydrocarbon combustion engine and for hypersonic aircraft with ramjet hydrogen combustion engine. Under using *QID*-method the fields of hydrodynamic parameters of subsonic coflowing jet were determined by using the simple algebraic method [11]. For the subsonic aircraft *B-747* we have taken into account the mixing between bypass flow and core flow. The results of *QID*-model calculations of the variation of the different species concentrations (in mole fractions) for the subsonic aircraft *B-747* ($M_e=0.8$; $H=10.7\text{ km}$) are presented in *Table 8*.

The fields of hydrodynamics parameters of hypersonic coflowing jet were determined by numerical solution parabolic equations for axisymmetric compressible turbulent flow by using second order numerical implicit scheme [12]. We considered flow behind hypersonic aircraft with aerodynamic scheme such as "Hotoll". This aircraft had only one exhaust and ogive form. The nonisobaric jet was replaced by a hypothetical isobaric jet. We used the two-equation turbulent model, that were taken into account the effect of compressibility to turbulent supersonic flows [13]. The results of calculations of temperature field in the hypersonic plume ($M_\infty=6$; $H=29\text{ km}$; $T_n=1800\text{ K}$, $P_n=P_\infty=13.9\text{ Pa}$) are presented in *Fig. 1*. The boundary conditions at the nozzle exit plane in this case were taken from nonequilibrium calculations by using *QID*-model in the internal flow of H_2 -combustion ramjet engine (see Performance Report). *Fig. 2* shows the changes averaged temperature, Mach number and radius of the plume along the plume of hypersonic

aircraft . The changes of mixture composition along the plume obtained by using *QID*-method in this case are presented in *Fig. 3*.

Under elaboration *2D*-model for calculations of nonequilibrium gas composition in plume of subsonic aircraft we have considered homogeneous co-flowing stream of air with constant velocity parallel to the jet axis and constant temperature, pressure and turbulent viscosity. The steady state set of isobaric jet mixing equations represent the relations for momentum balance, energy conservation, mass balance for the chemical species. The set of equations should be added by turbulence model equation. We used one equational model for eddy viscosity [14]. The implicit scheme is used.

Fig. 4 and *5* show the profiles of velocity U and temperature T at the nozzle exit plane of subsonic aircraft *B-747* ($M_\infty=0.8$; $H=10.7$ km) (boundary conditions at the nozzle exit plane for core flow were taken from *Table 5*). The changes of component concentrations across the plume at the different plane of plume ($x=10.6$ m, 99.2 m) in this case are presented in *Fig. 6, 7* correspondingly.

Summary

1. Our results show that under combustion of thermal destruction products of $n\text{-C}_8\text{H}_{18}$, and other hydrocarbon fuels with air at the equivalent ratio ~ 0.5 and less the chemical equilibrium is not realized at the exit plane of combustion chamber and in the gas turbine and nozzle for most of small components such as NO_2 , NO_3 , HNO , HNO_2 , HNO_3 , N_xH_y , HO_2 , OH . The chemical equilibrium is not realized in the internal flow of ramjet hydrogen combustion engine too.

So at the nozzle exit plane both of gas-turbine hydrocarbon combustion engine and of ramjet hydrogen combustion engine the relatively large values of concentration of such small components as NO_3 , HNO_2 , N_2O , HNO_3 , HNO , NH , N_2H , HO_2 , H_2O_2 may be realized. The exact definition of these component concentration as well as concentration of NO_x , OH , SO_2 , O , H , H_2 , H_2O at the nozzle exit plane is very important for plume chemistry.

2. The results which were obtained for subsonic and hypersonic aircrafts indicate on the considerable change of the composition of the gas mixture along the plume. This change can be caused not only by the mixture of combustion products with the atmosphere air but by proceeding of whole complex of nonequilibrium photochemical reactions. The photodissociation processes begin to influence on the formation of the free atoms and radicals at flight altitude $H \geq 18$ km. Neglect of these processes can result in essential (up to 10^4 times) mistakes of values γ_{OH} , γ_{O} , γ_{H} , γ_{HSO_3} and some products of CFC's disintegration. It was found that penetration of Cl-containing species from the atmosphere into the exhaust flow and its interaction with nitrogen oxides leads to essential increasing of the concentration of Cl , Cl_2 , ClO_2 , ClNO_3 , CH_3Cl and sometimes HCl and the decreasing of ClO concentration by comparison with background values. The results of our analysis show that the plume aircraft with both hydrocarbon and hydrogen combustion engine may be source of various pollutant components such as HNO , HNO_4 , ClO_2 , CH_3NO_2 , CH_3NO_3 , CH_2O , Cl , H_2O_2 , but not only NO , NO_2 , HNO_2 , HNO_3 , N_2O_5 , SO_2 , SO_3 , H_2SO_4 as it was supposed before [15, 16].

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Table 1. The reaction mechanism for the combustion of hydrocarbon (hydrogen)+air mixtures.

$$K_{\pm i} = A_i T^n \exp\left(\frac{E_{ai}}{T}\right) \quad (\text{cm}^3 / \text{mol})^{m-1} \cdot \text{s}^{-1}$$

| № | Reaction | K_+ | | | K_- | | | Source |
|---|--|----------|-------|----------|----------|------|----------|--------|
| | | A | n | E_{ai} | A | n | E_{ai} | |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| Reactions with H_2O , OH , O , H , H_2 , O_2 | | | | | | | | |
| 1. | $\text{H}_2\text{O}+\text{M}=\text{OH}+\text{H}+\text{M}$ | 1(24) | -2.2 | -59000 | 2.2(22) | -2 | 0 | [1] |
| 2. | $\text{H}_2+\text{M}=2\text{H}+\text{M}$ | 2.2(14) | 0 | -48300 | 9(17) | -1 | 0 | [1] |
| 3. | $\text{O}_2+\text{M}=2\text{O}+\text{M}$ | 2.6(18) | 0 | -59580 | 1.1(14) | -1 | 900 | [1] |
| 4. | $\text{OH}+\text{M}=\text{H}+\text{O}+\text{M}$ | 8.5(18) | -1 | -50830 | 7.1(18) | -1 | 0 | [1] |
| 5. | $\text{O}_2+\text{H}=\text{OH}+\text{O}$ | 2.2(14) | 0 | -8455 | 1.3(13) | 0 | -350 | [1] |
| 6. | $\text{H}_2+\text{O}=\text{OH}+\text{H}$ | 1.8(10) | 1 | -4480 | 8.3(9) | 1 | -3500 | [1] |
| 7. | $\text{H}_2\text{O}+\text{H}=\text{OH}+\text{H}_2$ | 8.4(13) | 0 | -10116 | 2(13) | 0 | -2600 | [1] |
| 8. | $\text{H}_2\text{O}+\text{O}=2\text{OH}$ | 5.8(13) | 0 | -9059 | 5.3(12) | 0 | -503 | [1] |
| 9. | $\text{H}_2+\text{O}_2=2\text{OH}$ | 1.7(15) | 0 | -24200 | 1.7(13) | 0 | -24100 | [1] |
| Reactions with HO_2 | | | | | | | | |
| 10. | $\text{HO}_2+\text{M}=\text{H}+\text{O}_2+\text{M}$ | 2.1(15) | 0 | -23000 | 1.5(15) | 0 | 500 | [1] |
| 11. | $\text{H}_2+\text{O}_2=\text{H}+\text{HO}_2$ | 1.9(13) | 0 | -24100 | 1.3(13) | 0 | 0 | [1] |
| 12. | $\text{H}_2\text{O}+\text{O}=\text{H}+\text{HO}_2$ | 4.76(11) | 0.372 | -28743 | 1(13) | 0 | -540 | [1] |
| 13. | $\text{H}_2\text{O}+\text{O}_2=\text{OH}+\text{HO}_2$ | 1.5(15) | 0.5 | -36600 | 3(14) | 0 | 0 | [1] |
| 14. | $\text{H}_2\text{O}+\text{OH}=\text{H}_2+\text{HO}_2$ | 7.2(9) | 0.43 | -36100 | 6.5(11) | 0 | -9400 | [1] |
| 15. | $2\text{OH}=\text{H}+\text{HO}_2$ | 1.2(13) | 0 | -20200 | 2.5(14) | 0 | -950 | [1] |
| 16. | $\text{OH}+\text{O}_2=\text{O}+\text{HO}_2$ | 1.3(13) | 0 | -28200 | 5(13) | 0 | -500 | [1] |
| Reactions with H_2O_2 | | | | | | | | |
| 17. | $\text{H}_2\text{O}_2+\text{M}=\text{OH}+\text{OH}+\text{M}$ | 1.2(17) | 0 | -22900 | 9.1(14) | 0 | 2650 | [1] |
| 18. | $\text{H}+\text{H}_2\text{O}_2=\text{HO}_2+\text{H}_2$ | 1.7(12) | 0 | -1900 | 6(11) | 0 | -9300 | [1] |
| 19. | $\text{H}+\text{H}_2\text{O}_2=\text{H}_2\text{O}+\text{OH}$ | 5(14) | 0 | -5000 | 2.4(14) | 0 | -40500 | [1] |
| 20. | $2\text{HO}_2=\text{H}_2\text{O}_2+\text{O}_2$ | 1.8(13) | 0 | -500 | 3(13) | 0 | -21600 | [1] |
| 21. | $\text{HO}_2+\text{H}_2\text{O}=\text{H}_2\text{O}_2+\text{OH}$ | 1.8(13) | 0 | -15100 | 1(13) | 0 | -910 | [1] |
| 22. | $\text{OH}+\text{HO}_2=\text{H}_2\text{O}_2+\text{O}$ | 5.2(10) | 0.5 | -10600 | 2(13) | 0 | -2950 | [1] |
| 23. | $\text{H}_2\text{O}+\text{O}_2=\text{H}_2\text{O}_2+\text{O}$ | 3.4(15) | 0.5 | -44800 | 8.4(11) | 0 | -2130 | [1] |
| Reactions with CH_4 , CH_3 , HCO , CO , CH_2O , CH_3O | | | | | | | | |
| 24. | $\text{CH}_4+\text{H}=\text{CH}_3+\text{H}_2$ | 7.59(14) | 0 | -7993 | 2(13) | 0 | -7212 | [1] |
| 25. | $\text{CH}_4+\text{O}=\text{CH}_3+\text{OH}$ | 2.14(6) | 2.2 | -3266 | 3.55(4) | 2.2 | -1976 | [1] |
| 26. | $\text{CH}_2\text{O}+\text{M}=\text{HCO}+\text{H}+\text{M}$ | 3.31(16) | 0 | -40824 | 1.41(11) | 1 | 5947 | [1] |
| 27. | $\text{CH}_2\text{O}+\text{O}_2=\text{HO}_2+\text{HCO}$ | 3.63(15) | 0 | -23204 | 1(14) | 0 | -1512 | [1] |
| 28. | $\text{CH}_2\text{O}+\text{O}=\text{HCO}+\text{OH}$ | 5.01(13) | 0 | -2318 | 1.74(12) | 0 | -8654 | [1] |
| 29. | $\text{CH}_2\text{O}+\text{OH}=\text{HCO}+\text{H}_2\text{O}$ | 3.47(9) | 1.2 | 242 | 1.18(9) | 1.2 | -14802 | [1] |
| 30. | $\text{HCO}+\text{M}=\text{H}+\text{CO}+\text{M}$ | 3.47(17) | -1 | -8568 | 5.01(11) | 1 | -781 | [1] |
| 31. | $\text{HCO}+\text{H}_2=\text{CH}_2\text{O}+\text{H}$ | 2.63(13) | 0 | -12686 | 5.01(13) | 0 | -2016 | [1] |
| 32. | $\text{HCO}+\text{O}_2=\text{HO}_2+\text{CO}$ | 3.02(12) | 0 | 0 | 8.91(12) | 0 | -16274 | [1] |
| 33. | $\text{HCO}+\text{H}=\text{H}_2+\text{CO}$ | 1.2(14) | 0 | 0 | 1.32(15) | 0 | -45360 | [1] |
| 34. | $\text{HCO}+\text{O}=\text{OH}+\text{CO}$ | 1(14) | 0 | 0 | 2.88(14) | 0 | -44302 | [1] |
| 35. | $\text{HCO}+\text{OH}=\text{H}_2\text{O}+\text{CO}$ | 3.16(13) | 0 | 0 | 8.91(14) | 0 | -52970 | [1] |
| 36. | $2\text{HCO}=\text{CH}_2\text{O}+\text{CO}$ | 1.81(13) | 0 | 0 | | | | [2] |
| 37. | $2\text{HCO}=\text{H}_2+2\text{CO}$ | 3.01(12) | 0 | 0 | | | | [2] |
| 38. | $\text{CH}_4+\text{M}=\text{CH}_3+\text{H}+\text{M}$ | 1.41(17) | 0 | -44554 | 2.82(11) | 1 | 9828 | [6] |
| 39. | $\text{CH}_3+\text{O}=\text{CH}_2\text{O}+\text{H}$ | 1.29(14) | 0 | -1008 | 1.7(15) | 0 | -36102 | [6] |
| 40. | $\text{CH}_3+\text{OH}=\text{CH}_2\text{O}+\text{H}_2$ | 7.94(12) | 0 | 0 | 1.2(14) | 0 | -36147 | [6] |
| 41. | $\text{CH}_3+\text{HO}_2=\text{CH}_3\text{O}+\text{OH}$ | 1.99(13) | 0 | 0 | | | | [2] |
| 42. | $\text{CH}_3+\text{HO}_2=\text{CH}_4+\text{O}_2$ | 1(12) | 0 | -202 | 7.59(13) | 0 | -29529 | [6] |
| 43. | $\text{CH}_3+\text{H}_2\text{O}=\text{CH}_4+\text{OH}$ | 4.79(2) | 2.9 | -7489 | 1.59(5) | 2.4 | -1063 | [6] |
| 44. | $\text{CH}_3+\text{CH}_2\text{O}=\text{CH}_4+\text{HCO}$ | 5.54(3) | 2.81 | -2950 | 7.28(3) | 2.85 | -11330 | [2] |
| 45. | $\text{CH}_3+\text{HCO}=\text{CH}_4+\text{CO}$ | 1.2(14) | 0 | 0 | 5.13(13) | 0.5 | -45597 | [2] |
| 46. | $\text{CH}_3+\text{O}_2=\text{CH}_3\text{O}+\text{O}$ | 1.99(18) | -1.57 | -14710 | | | | [2] |
| 47. | $\text{CH}_3\text{O}+\text{M}=\text{CH}_2\text{O}+\text{H}+\text{M}$ | 3.91(37) | -6.65 | -16740 | | | | [2] |
| 48. | $\text{CH}_3\text{O}+\text{O}_2=\text{CH}_2\text{O}+\text{HO}_2$ | 6.62(10) | 0 | -1310 | | | | [2] |
| 49. | $\text{CH}_3\text{O}+\text{H}=\text{CH}_2\text{O}+\text{H}_2$ | 1.99(13) | 0 | 0 | | | | [2] |
| 50. | $\text{CH}_3\text{O}+\text{O}=\text{CH}_2\text{O}+\text{OH}$ | 6.02(12) | 0 | 0 | | | | [2] |
| 51. | $\text{CH}_3\text{O}+\text{OH}=\text{CH}_2\text{O}+\text{H}_2\text{O}$ | 1.81(13) | 0 | 0 | | | | [2] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|----------|------|--------|----------|------|--------|-----|
| 52. | $\text{CH}_3\text{O}+\text{CH}_3=\text{CH}_2\text{O}+\text{CH}_4$ | 2.41(13) | 0 | 0 | | | | [2] |
| 53. | $\text{CH}_3+\text{O}_2=\text{CH}_2\text{O}+\text{OH}$ | 3(10) | 0 | -5040 | | | | [6] |
| 54. | $\text{CH}_2\text{O}+\text{HO}_2=\text{H}_2\text{O}_2+\text{HCO}$ | 2(11) | 0 | -4032 | 2.19(10) | 0 | -3321 | [6] |
| 55. | $\text{CH}_3\text{O}+\text{HO}_2=\text{CH}_2\text{O}+\text{H}_2\text{O}_2$ | 3.01(11) | 0 | 0 | | | | [2] |
| 56. | $\text{CH}_3+\text{H}_2\text{O}_2=\text{CH}_4+\text{HO}_2$ | 3.72(10) | 0 | -645 | 1.12(13) | 0 | -10312 | [6] |
| Reactions with CO_2 , C, CH, CH_2 | | | | | | | | |
| 57. | $\text{CO}+\text{O}_2=\text{CO}_2+\text{O}$ | 3.16(11) | 0 | -18950 | 2.75(12) | 0 | -22090 | [6] |
| 58. | $\text{CO}_2+\text{M}=\text{CO}+\text{O}+\text{M}$ | 5.5(21) | -1 | -66427 | 5.89(15) | 0 | -2066 | [6] |
| 59. | $\text{CO}+\text{OH}=\text{H}+\text{CO}_2$ | 1.51(7) | 1.3 | 388 | 1.7(9) | 1.3 | -10876 | [6] |
| 60. | $\text{CO}+\text{HO}_2=\text{OH}+\text{CO}_2$ | 1.51(14) | 0 | -11920 | 1.7(15) | 0 | -43092 | [6] |
| 61. | $\text{HCO}+\text{O}=\text{H}+\text{CO}_2$ | 3.01(13) | 0 | 0 | | | | [2] |
| 62. | $\text{CH}_3+\text{M}=\text{CH}_2+\text{H}+\text{M}$ | 2.51(16) | 0 | -47917 | | | | [6] |
| 63. | $\text{CH}_3+\text{M}=\text{CH}+\text{H}_2+\text{M}$ | 1(16) | 0 | -45313 | | | | [6] |
| 64. | $\text{CH}_3\text{O}+\text{CO}=\text{CH}_3+\text{CO}_2$ | 1.57(13) | 0 | -5940 | | | | [2] |
| 65. | $\text{CH}+\text{M}=\text{C}+\text{H}+\text{M}$ | 3.16(14) | 0 | -37500 | | | | [6] |
| 66. | $\text{CH}+\text{H}=\text{C}+\text{H}_2$ | 1.58(14) | 0 | 0 | 8.3(14) | 0 | -12760 | [6] |
| 67. | $\text{CH}+\text{O}_2=\text{CO}+\text{OH}$ | 1.35(11) | 0.67 | -13385 | 5.13(11) | 0.67 | -96667 | [6] |
| 68. | $\text{CH}+\text{O}_2=\text{HCO}+\text{O}$ | 1(13) | 0 | 0 | 1.35(13) | 0 | -37474 | [6] |
| 69. | $\text{CH}_2+\text{M}=\text{CH}+\text{H}+\text{M}$ | 3.98(15) | 0 | -47396 | | | | [6] |
| 70. | $\text{CH}_2+\text{M}=\text{C}+\text{H}_2+\text{M}$ | 3.16(14) | 0 | -35938 | | | | [6] |
| 71. | $\text{CH}_2+\text{O}=\text{CH}+\text{OH}$ | 1.91(11) | 0.68 | -13021 | 5.9(10) | 0.68 | -13245 | [6] |
| 72. | $\text{CH}_2+\text{OH}=\text{CH}+\text{H}_2\text{O}$ | 2.69(11) | 0.67 | -13385 | 8.13(11) | 0.67 | -22854 | [6] |
| Reactions with CH_2OH , CH_3OH , CH_3O_2 , CH_3OOH | | | | | | | | |
| 73. | $\text{CH}_3\text{OH}+\text{OH}=\text{CH}_2\text{OH}+\text{H}_2\text{O}$ | 3.16(4) | 2.65 | 458 | 1.86(7) | 1.66 | -13182 | [6] |
| 74. | $\text{CH}_3\text{OH}+\text{O}=\text{CH}_2\text{OH}+\text{OH}$ | 1.7(12) | 0 | -1193 | 7.94(5) | 1.66 | -4349 | [6] |
| 75. | $\text{CH}_3\text{OH}+\text{H}=\text{CH}_2\text{OH}+\text{H}_2$ | 3.02(13) | 0 | -3646 | 3.24(7) | 1.66 | -7896 | [6] |
| 76. | $\text{CH}_3\text{OH}+\text{H}=\text{CH}_3+\text{H}_2\text{O}$ | 5.25(12) | 0 | -2781 | 2.09(12) | 0 | -19245 | [6] |
| 77. | $\text{CH}_3\text{OH}+\text{CH}_3=\text{CH}_2\text{OH}+\text{CH}_4$ | 1.82(11) | 0 | -5104 | 5.01(6) | 1.66 | -9600 | [6] |
| 78. | $\text{CH}_3\text{OH}+\text{HO}_2=\text{CH}_2\text{OH}+\text{H}_2\text{O}_2$ | 6.31(12) | 0 | -10083 | 1(7) | 1.66 | -5958 | [6] |
| 79. | $\text{CH}_3\text{OH}+\text{M}=\text{CH}_3+\text{OH}+\text{M}$ | 3.02(18) | 0 | -40320 | 1.45(13) | 0 | 5494 | [6] |
| 80. | $\text{CH}_2\text{OH}+\text{M}=\text{CH}_2\text{O}+\text{H}+\text{M}$ | 2.09(14) | 0 | -12708 | 4.9(16) | -0.7 | -3948 | [6] |
| 81. | $\text{CH}_2\text{OH}+\text{O}_2=\text{CH}_2\text{O}+\text{HO}_2$ | 1(12) | 0 | -3438 | 8.71(17) | -1.7 | -14750 | [6] |
| 82. | $\text{CH}_3\text{O}_2+\text{OH}=\text{CH}_3\text{OH}+\text{O}_2$ | 6.02(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 83. | $2\text{CH}_3\text{O}_2=\text{CH}_3\text{OH}+\text{CH}_2\text{O}+\text{O}_2$ | 1.26(11) | 0 | 0 | 0 | 0 | 0 | [2] |
| 84. | $\text{CH}_3\text{O}+\text{CH}_4=\text{CH}_3\text{OH}+\text{CH}_3$ | 1.57(11) | 0 | -4450 | | | | [2] |
| 85. | $\text{CH}_3\text{O}+\text{CH}_2\text{O}=\text{CH}_3\text{OH}+\text{HCO}$ | 1.02(11) | 0 | -1500 | | | | [2] |
| 86. | $\text{CH}_3\text{O}+\text{HCO}=\text{CH}_3\text{OH}+\text{CO}$ | 9.03(13) | 0 | 0 | | | | [2] |
| 87. | $\text{CH}_3\text{O}_2+\text{M}=\text{CH}_3+\text{O}_2+\text{M}$ (*) | 7.22(48) | -10 | -16731 | 9.03(58) | -15 | -8567 | [2] |
| 88. | $\text{CH}_3\text{O}_2+\text{H}_2=\text{CH}_3\text{OOH}+\text{H}$ | 3.01(13) | 0 | -13100 | 0 | 0 | 0 | [2] |
| 89. | $\text{CH}_3\text{O}_2+\text{H}=\text{CH}_3\text{O}+\text{OH}$ | 9.63(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 90. | $\text{CH}_3\text{O}_2+\text{O}=\text{CH}_3\text{O}+\text{O}_2$ | 3.61(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 91. | $\text{CH}_3\text{O}_2+\text{HO}_2=\text{CH}_3\text{OOH}+\text{O}_2$ | 4.64(10) | 0 | 1310 | 3.01(12) | 0 | -19656 | [5] |
| 92. | $\text{CH}_3\text{O}_2+\text{H}_2\text{O}_2=\text{CH}_3\text{OOH}+\text{HO}_2$ | 2.41(12) | 0 | -5000 | 0 | 0 | 0 | [2] |
| 93. | $\text{CH}_3\text{O}_2+\text{CH}_4=\text{CH}_3\text{OOH}+\text{CH}_3$ | 1.81(11) | 0 | -9300 | 0 | 0 | 0 | [2] |
| 94. | $\text{CH}_3\text{O}_2+\text{CH}_2\text{O}=\text{CH}_3\text{OOH}+\text{HCO}$ | 1.3(11) | 0 | -4536 | 2.5(10) | 0 | -5090 | [5] |
| 95. | $\text{CH}_3\text{O}_2+\text{HCO}=\text{CH}_3\text{O}+\text{H}+\text{CO}_2$ | 3.01(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 96. | $\text{CH}_3\text{O}_2+\text{CH}_3=\text{CH}_3\text{O}+\text{CH}_3\text{O}$ | 3.8(12) | 0 | 605 | 2.4(10) | 0 | 0 | [5] |
| 97. | $2\text{CH}_3\text{O}_2=2\text{CH}_3\text{O}+\text{O}_2$ | 7.83(10) | 0 | 0 | 0 | 0 | 0 | [2] |
| 98. | $\text{CH}_3\text{O}+\text{CH}_3\text{O}_2=\text{CH}_2\text{O}+\text{CH}_3\text{OOH}$ | 3.01(11) | 0 | 0 | 0 | 0 | 0 | [2] |
| 99. | $\text{CH}_3\text{OOH}+\text{M}=\text{CH}_3\text{O}+\text{OH}+\text{M}$ | 6.46(14) | 0 | -21672 | 1(11) | 0 | 0 | [5] |
| 100. | $\text{CH}_3\text{OOH}+\text{OH}=\text{CH}_3\text{O}_2+\text{H}_2\text{O}$ | 3.24(13) | 0 | -504 | 3.02(13) | 0 | -16531 | [5] |
| 101. | $\text{CH}_3\text{O}_2+\text{CH}_3\text{OH}=\text{CH}_2\text{OH}+\text{CH}_3\text{OOH}$ | 6.31(12) | 0 | -9757 | 1(9) | 0 | -5040 | [5] |
| Reactions with C_2 , C_2H_y , CH_2CO , CH_3CO , CH_3CHO , CH_3OOCH_3 , C_2HO | | | | | | | | |
| 102. | $\text{C}_2\text{H}_6(+\text{M})=2\text{CH}_3(+\text{M})$ | 4.27(19) | -1 | -44633 | 1.66(13) | 0 | 157 | [5] |
| 103. | $\text{C}_2\text{H}_5+\text{H}=\text{C}_2\text{H}_6$ (**) | | | | 0 | 0 | 0 | [2] |
| 104. | $\text{C}_2\text{H}_5+\text{HO}_2=\text{C}_2\text{H}_6+\text{O}_2$ | 3.01(11) | 0 | 0 | 4.03(13) | 0 | -25600 | [2] |
| 105. | $\text{C}_2\text{H}_5+\text{H}_2=\text{C}_2\text{H}_6+\text{H}$ | 3.07 | 3.6 | -4253 | 5.54(2) | 3.5 | -2600 | [2] |
| 106. | $\text{C}_2\text{H}_6+\text{O}=\text{C}_2\text{H}_5+\text{OH}$ | 1.12(14) | 0 | -3956 | 2.09(13) | 0 | -6411 | [6] |
| 107. | $\text{C}_2\text{H}_5+\text{H}_2\text{O}=\text{C}_2\text{H}_6+\text{OH}$ | 3.37(6) | 1.44 | -10150 | 8.85(9) | 1.04 | -913 | [2] |
| 108. | $\text{C}_2\text{H}_5+\text{H}_2\text{O}_2=\text{C}_2\text{H}_6+\text{HO}_2$ | 8.43(9) | 0 | -490 | 2.95(11) | 0 | -7520 | [2] |
| 109. | $\text{C}_2\text{H}_6+\text{CH}_3=\text{C}_2\text{H}_5+\text{CH}_4$ | 5.48(-1) | 4 | -4169 | 8.43(-2) | 4.1 | -6322 | [2] |
| 110. | $\text{C}_2\text{H}_5+\text{HCO}=\text{C}_2\text{H}_6+\text{CO}$ | 1.2(14) | 0 | 0 | | | | [2] |
| 111. | $\text{C}_2\text{H}_6+\text{HCO}=\text{C}_2\text{H}_5+\text{CH}_2\text{O}$ | 4.7(4) | 2.7 | -9176 | 5.48(3) | 2.8 | -2950 | [2] |
| 112. | $\text{C}_2\text{H}_5+\text{CH}_3\text{O}=\text{C}_2\text{H}_6+\text{CH}_2\text{O}$ | 2.4(13) | 0 | 0 | | | | [2] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------|---------------------------------------|----------|-------|--------|----------|-------|--------|-----|
| 113. | $C_2H_6+CH_3O=C_2H_5+CH_3OH$ | 2.4(11) | 0 | -3570 | | | | [2] |
| 114. | $C_2H_6+CH_3O_2=C_2H_5+CH_3O_2H$ | 2.95(11) | 0 | -7520 | 0 | 0 | 0 | [2] |
| 115. | $C_2H_6+CH_3CO=C_2H_5+CH_3CHO$ | 1.8(4) | 2.75 | -8820 | 0 | 0 | 0 | [2] |
| 116. | $C_2H_5+C_2H_2=C_2H_6+C_2H$ | 2.7(11) | 0 | -11800 | 3.6(12) | 0 | 0 | [2] |
| 117. | $C_2H_5+C_2H_3=C_2H_6+C_2H_2$ | 4.8(11) | 0 | 0 | | | | [2] |
| 118. | $C_2H_5+C_2H_4=C_2H_6+C_2H_3$ | 6.6(2) | 3.1 | -9063 | 6.02(2) | 3.3 | -5285 | [2] |
| 119. | $2C_2H_5=C_2H_6+C_2H_4$ | 1.38(12) | 0 | 0 | | | | [2] |
| 120. | $C_2H_5(+M)=C_2H_4+H(+M)$ | 1.07(18) | -1 | -21783 | 2.19(13) | 0 | -1046 | [5] |
| 121. | $C_2H_5+O_2=C_2H_4+HO_2$ | 8.4(11) | 0 | -1950 | | | | [2] |
| 122. | $C_2H_5+O_2=C_2H_5O_2$ | 1(12) | 0 | 0 | 4.37(18) | -1 | -18711 | [5] |
| 123. | $C_2H_5+H=2CH_3$ | (**) | | | | | | [2] |
| 124. | $C_2H_4+H_2=C_2H_5+H$ | 1(13) | 0 | -34300 | 1.8(12) | 0 | 0 | [2] |
| 125. | $C_2H_5+O=CH_3CHO+H$ | 8(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 126. | $C_2H_5+O=CH_2O+CH_3$ | 1.6(13) | 0 | 0 | | | | [2] |
| 127. | $C_2H_5+OH=C_2H_4+H_2O$ | 2.4(13) | 0 | 0 | | | | [2] |
| 128. | $C_2H_5+OH=CH_3+H+CH_2O$ | 2.4(13) | 0 | 0 | | | | [2] |
| 129. | $C_2H_5+HO_2=CH_3+CH_2O+OH$ | 2.4(13) | 0 | 0 | | | | [2] |
| 130. | $C_2H_5+HO_2=C_2H_5O+OH$ | 3.24(13) | 0 | 0 | 2(10) | 0 | 0 | [5] |
| 131. | $C_2H_5+HO_2=C_2H_4+H_2O_2$ | 3(11) | 0 | 0 | | | | [2] |
| 132. | $C_2H_5+CH_3=CH_4+C_2H_4$ | 1.96(13) | -0.5 | 0 | | | | [2] |
| 133. | $C_2H_5+CH_3O_2=C_2H_5O+CH_3O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 134. | $C_2H_5+C_2H=C_2H_4+C_2H_2$ | 1.8(12) | 0 | 0 | 0 | 0 | 0 | [2] |
| 135. | $2C_2H_4=C_2H_3+C_2H_5$ | 4.8(14) | 0 | -36000 | 4.8(11) | 0 | 0 | [2] |
| 136. | $C_2H_5O=CH_3+CH_2O$ | 1(15) | 0 | -10917 | 2(5) | 1 | -4963 | [5] |
| 137. | $C_2H_5O+O_2=CH_3CHO+HO_2$ | 1.82(11) | 0 | -930 | 4.68(9) | 0 | -15168 | [5] |
| 138. | $C_2H_5O_2+HO_2=C_2H_5O+OH+O_2$ | 1(12) | 0 | 0 | | 0 | 0 | [5] |
| 139. | $C_2H_5O_2+HO_2=C_2H_5O_2H+O_2$ | 4.57(10) | 0 | 1314 | 3.02(12) | 0 | -19711 | [5] |
| 140. | $C_2H_5O_2+CH_4=C_2H_5O_2H+CH_3$ | 1.12(13) | 0 | -10341 | 7.6(11) | 0 | -647 | [5] |
| 141. | $C_2H_5O_2+CH_2O=C_2H_5O_2H+HCO$ | 1.29(11) | 0 | -4549 | 2.51(10) | 0 | -5105 | [5] |
| 142. | $C_2H_5O_2+CH_3OH=C_2H_5O_2H+CH_2OH$ | 6.31(12) | 0 | -9785 | 1(9) | 0 | -5054 | [5] |
| 143. | $C_2H_5O_2+C_2H_4=C_2H_5O_2H+C_2H_3$ | 7.08(11) | 0 | -8648 | 2(10) | 0 | -7581 | [5] |
| 144. | $C_2H_5O_2+CH_3CHO=C_2H_5O_2H+CH_3CO$ | 1.15(11) | 0 | -5054 | 5.01(9) | 0 | -5105 | [5] |
| 145. | $C_2H_5O_2H=C_2H_5O+OH$ | 6.46(14) | 0 | -21733 | 1(10) | 0 | 0 | [5] |
| 146. | $C_2H_5O_2H+O=C_2H_5O_2+OH$ | 1.99(13) | 0 | -2390 | 0 | 0 | 0 | [7] |
| 147. | $C_2H_5O_2H+OH=C_2H_5O_2+H_2O$ | 1.8(12) | 0 | 190 | 0 | 0 | 0 | [7] |
| 148. | $C_2H_4+M=C_2H_2+H_2+M$ | 2.57(17) | 0 | -39957 | 4.17(10) | 1 | -18406 | [6] |
| 149. | $C_2H_4+M=C_2H_3+H+M$ | 3.8(17) | 0 | -51125 | 2(17) | 0 | 0 | [6] |
| 150. | $C_2H_4+O_2=C_2H_3+HO_2$ | 4.2(13) | 0 | -29000 | | | | [2] |
| 151. | $C_2H_4+H=C_2H_3+H_2$ | 1.32(6) | 2.5 | -6160 | 3(4) | 2.6 | -4298 | [2] |
| 152. | $C_2H_4+O=CH_3+HCO$ | 1.32(8) | -1.6 | -215 | | | | [2] |
| 153. | $C_2H_4+O=CH_2O+CH_2$ | 2.5(13) | 0 | -2604 | 3(12) | 0 | -8167 | [6] |
| 154. | $C_2H_4+OH=CH_3+CH_2O$ | 2(12) | 0 | -500 | 6(11) | 0 | -8583 | [6] |
| 155. | $C_2H_4+OH=C_2H_3+H_2O$ | 1.56(4) | 2.8 | -2100 | 4.8(2) | 2.9 | -7480 | [2] |
| 156. | $C_2H_4+HO_2=CH_3CHO+OH$ | 6(9) | 0 | -4000 | 9(13) | 0 | 0 | [2] |
| 157. | $C_2H_3+H_2O_2=C_2H_4+HO_2$ | 1.2(10) | 0 | 300 | | | | [2] |
| 158. | $C_2H_4+CH_3=C_2H_3+CH_4$ | 6.6 | 3.7 | -4780 | 1.44 | 4 | -2754 | [2] |
| 159. | $C_2H_4+CO=C_2H_3+HCO$ | 1.5(14) | 0 | -45600 | | | | [2] |
| 160. | $C_2H_3+CH_2O=C_2H_4+HCO$ | 5.4(3) | 2.8 | -2950 | | | | [2] |
| 161. | $C_2H_3+CH_3O=C_2H_4+CH_2O$ | 2.4(13) | 0 | 0 | | | | [2] |
| 162. | $C_2H_4+CH_3O_2=C_2H_3+CH_3O_2H$ | 7.08(11) | 0 | -8623 | 2(10) | 0 | -7560 | [5] |
| 163. | $2C_2H_3=C_2H_4+C_2H_2$ | 9.6(11) | 0 | 0 | | | | [2] |
| 164. | $C_2H_4+CH_3CO_3=C_2H_3+CH_3CO_3H$ | 7.08(11) | 0 | -8648 | 2(10) | 0 | -7581 | [5] |
| 165. | $C_2H_3+M=C_2H_2+H+M$ | 4.15(41) | -7.49 | -22917 | 6.03(16) | -7.27 | -3632 | [2] |
| 166. | $C_2H_3+O_2=C_2H_2+HO_2$ | 1.2(11) | 0 | 0 | | | | [2] |
| 167. | $C_2H_3+H=C_2H_2+H_2$ | 9.6(13) | 0 | 0 | 2.4(12) | 0 | -32700 | [2] |
| 168. | $C_2H_3+O=CH_2CO+H$ | 9.6(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 169. | $C_2H_3+OH=H_2O+C_2H_2$ | 3(13) | 0 | 0 | | | | [2] |
| 170. | $CH_3CHO=C_2H_3+OH$ | 0 | 0 | 0 | 3(13) | 0 | 0 | [2] |
| 171. | $C_2H_3+HO_2=OH+CH_3+CO$ | 3(13) | 0 | 0 | | | | [2] |
| 172. | $C_2H_3+CH_3=C_2H_2+CH_4$ | 3.9(11) | 0 | 0 | | | | [2] |
| 173. | $2C_2H_2=C_2H_3+C_2H$ | 9.6(12) | 0 | -42500 | 9.6(11) | 0 | 0 | [2] |
| 174. | $C_2H_2+M=C_2H+H+M$ | 3.02(16) | 0 | -54432 | 1.78(11) | 1 | 9778 | [6] |
| 175. | $C_2H_2+O_2=2HCO$ | 4(12) | 0 | -14583 | 1(11) | 0 | -33151 | [6] |
| 176. | $C_2H_2+O_2=C_2H+HO_2$ | 1.2(13) | 0 | -37500 | 1.8(13) | 0 | 0 | [2] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------------------------|-------------------------------------|--------------|--------|--------|----------|-------|--------|-----|
| 177. | $C_2H_2+H=C_2H+H_2$ | 6(13) | 0 | -11200 | 1.14(13) | 0 | -1450 | [2] |
| 178. | $C_2H_2+O=CH_2+CO$ | (**) | | | 3.13(13) | 0 | 0 | [2] |
| 179. | $C_2H_2+O=C_2HO+H$ | 9(12) | 0 | -2285 | 0 | 0 | 0 | [2] |
| 180. | $C_2H+OH=C_2H_2+O$ | 1.8(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 181. | $C_2H_2+OH=C_2H+H_2O$ | 1.44(4) | 2.68 | -6060 | 0 | 0 | 0 | [2] |
| 182. | $C_2H_2+OH=CH_3+CO$ | 1.2(12) | 0 | -260 | 2.51(12) | 0 | -29232 | [6] |
| 183. | $C_2H_2+OH=CH_2CO+H$ | 3.16(11) | 0 | -101 | 3.16(12) | 0 | -10518 | [5] |
| 184. | $C_2H_2+HO_2=CH_2CO+OH$ | 6(9) | 0 | -4000 | 0 | 0 | 0 | [2] |
| 185. | $C_2H_2+CH_3=CH_4+C_2H$ | 1.8(11) | 0 | -8700 | 1.8(12) | 0 | -250 | [2] |
| 186. | $C_2H_2+CO=C_2H+HCO$ | 4.8(14) | 0 | -53700 | 6(13) | 0 | 0 | [2] |
| 187. | $C_2H+CH_3O=C_2H_2+CH_2O$ | 2.4(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 188. | $2C_2H=C_2H_2+C_2$ | 1.8(12) | 0 | 0 | | | | [2] |
| 189. | $C_2H+O_2=CO+HCO$ | 1(13) | 0 | -3528 | 8.51(12) | 0 | -68754 | [5] |
| 190. | $C_2H+O_2=C_2HO+O$ | 6(11) | 0 | 0 | 0 | 0 | 0 | [2] |
| 191. | $C_2H+H=C_2+H_2$ | 3.6(13) | 0 | -14223 | | | | [2] |
| 192. | $C_2H+O=CH+CO$ | 5.01(13) | 0 | 0 | 3.16(13) | 0 | -29953 | [5] |
| 193. | $C_2H+OH=CH_2+CO$ | 1.8(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 194. | $C_2H+HO_2=C_2HO+OH$ | 1.8(13) | 0 | 0 | | | | [2] |
| 195. | $C_2H+CH_3O_2=C_2HO+CH_3O$ | 2.4(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 196. | $C_2HO+H=CH_2+CO$ | 1.1(14) | 0 | 0 | 6.61(13) | 0 | -19787 | [5] |
| 197. | $C_2HO+O=HCO+CO$ | 3.39(13) | 0 | -1008 | 8.32(13) | 0 | -64663 | [5] |
| 198. | $C_2HO+OH=2HCO$ | 1(13) | 0 | 0 | 4.79(13) | 0 | -20341 | [3] |
| 199. | $CH_2CO+H=CH_3+CO$ | 1.1(13) | 0 | -1714 | 2.4(12) | 0 | -20261 | [5] |
| 200. | $CH_2CO+O=2HCO$ | 1(13) | 0 | -1210 | 3.47(11) | 0 | -16884 | [5] |
| 201. | $CH_2CO+OH=CH_2O+HCO$ | 2.82(13) | 0 | 0 | 2.75(13) | 0 | -9324 | [5] |
| 202. | $CH_2CO+M=CH_2+CO+M$ | 2(16) | 0 | -30240 | 4.57(10) | 0 | 0 | [5] |
| 203. | $CH_2CO+O=C_2HO+OH$ | 5.01(13) | 0 | -4032 | 7.08(10) | 0 | -4032 | [5] |
| 204. | $CH_2CO+OH=C_2HO+H_2O$ | 7.6(12) | 0 | -1512 | 1(11) | 0 | -5544 | [5] |
| 205. | $CH_2CO+H=C_2HO+H_2$ | 7.6(13) | 0 | -4032 | 2.45(11) | 0 | -4032 | [5] |
| 206. | $CH_3CO+M=CH_3+CO+M$ | (*) 8.73(42) | -8.62 | -11284 | 2.4(14) | -7.56 | -5490 | [2] |
| 207. | $CH_3CO+O_2=CH_3CO_3$ | 1(10) | 0 | 1365 | 2.88(16) | -1 | -18852 | [5] |
| 208. | $CH_3CO+O=CH_3+CO_2$ | 9.6(12) | 0 | 0 | 0 | 0 | 0 | [2] |
| 209. | $CH_3CO+OH=CH_2CO+H_2O$ | 1.2(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 210. | $CH_3CO+OH=CH_3+CO+OH$ | 3(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 211. | $CH_3CO+H_2=CH_3CHO+H$ | 1.78(13) | 0 | -11925 | 3.98(13) | 0 | -2117 | [5] |
| 212. | $CH_3CO+HO_2=CH_3+CO_2+OH$ | 3(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 213. | $CH_3CO+H_2O_2=CH_3CHO+HO_2$ | 1(12) | 0 | -7106 | 1.7(12) | 0 | -5393 | [5] |
| 214. | $CH_3CO+CH_4=CH_3CHO+CH_3$ | 1.51(13) | 0 | -14334 | 1.74(12) | 0 | -4254 | [5] |
| 215. | $CH_3CO+HCO=CH_3CHO+CO$ | 9(12) | 0 | 0 | 0 | 0 | 0 | [2] |
| 216. | $CH_3CO+CH_2O=CH_3CHO+HCO$ | 1.8(11) | 0 | -6500 | 0 | 0 | 0 | [2] |
| 217. | $CH_3CO+CH_3O=CH_2CO+CH_3OH$ | 6(12) | 0 | 0 | 0 | 0 | 0 | [2] |
| 218. | $CH_3CO+CH_3O=CH_3CHO+CH_2O$ | 6(12) | 0 | 0 | 0 | 0 | 0 | [2] |
| 219. | $CH_3CO+CH_3O_2=CH_3+CO_2+CH_3O$ | 2.4(13) | 0 | 0 | 0 | 0 | 0 | [2] |
| 220. | $CH_3CHO=CH_3+HCO$ | 7.08(15) | 0 | -41294 | 3.8(9) | 1 | 0 | [5] |
| 221. | $CH_3CHO+O_2=CH_3CO+HO_2$ | 2(13) | 0.5 | -21269 | 1(7) | 0.5 | -2016 | [5] |
| 222. | $CH_3CHO+O=CH_3CO+OH$ | 5.01(12) | 0 | -902 | 1(12) | 0 | -9657 | [5] |
| 223. | $CH_3CHO+OH=CH_3CO+H_2O$ | 1(13) | 0 | 0 | 1.91(13) | 0 | -18456 | [5] |
| 224. | $CH_3CHO+CH_3O=CH_3CO+CH_3OH$ | 1.15(11) | 0 | -645 | 3.02(11) | 0 | -9374 | [5] |
| 225. | $CH_3CHO+CH_3O_2=CH_3CO+CH_3O_2H$ | 1.15(11) | 0 | -5040 | 5.01(9) | 0 | -5090 | [5] |
| 226. | $2CH_3O_2=CH_3O_2CH_3+O_2$ | 5.01(11) | 0 | -1008 | 0 | 0 | 0 | [2] |
| 227. | $CH_3O_2CH_3=2CH_3O$ | 3.02(15) | 0 | -18648 | 1.8(12) | 0 | 0 | [2] |
| 228. | $CH_3CO_3+HO_2=CH_3CO_3H+O_2$ | 1(12) | 0 | 0 | 3.98(13) | 0 | -25776 | [5] |
| 229. | $CH_3CO_3+CH_4=CH_3CO_3H+CH_3$ | 1.12(13) | 0 | -10341 | 7.6(11) | 0 | -647 | [5] |
| 230. | $CH_3CO_3+CH_2O=CH_3CO_3H+HCO$ | 1(12) | 0 | -5337 | 1(11) | 0 | -5054 | [5] |
| 231. | $CH_3CO_3+CH_3OH=CH_3CO_3H+CH_2OH$ | 6.31(12) | 0 | -9785 | 1(9) | 0 | -5054 | [5] |
| 232. | $CH_3CO_3+CH_3CHO=CH_3CO_3H+CH_3CO$ | 1.2(11) | 0 | -2476 | 2(10) | 0 | -5054 | [5] |
| 233. | $CH_3CO_3H=CH_3+CO_2+OH$ | 2(14) | 0 | -20292 | 0 | 0 | 0 | [5] |
| Reactions with C_3H_7 | | | | | | | | |
| 234. | $C_3H_8=C_2H_5+CH_3$ | 1.7(16) | 0 | -42879 | 1.51(10) | 1 | 162 | [3] |
| 235. | $C_3H_8=nC_3H_7+H$ | 7.55(15) | -0.344 | -50301 | 2(13) | 0 | 0 | [8] |
| 236. | $C_3H_8=iC_3H_7+H$ | 7.16(14) | -0.299 | -48135 | 2(13) | 0 | 0 | [8] |
| 237. | $C_3H_8+O_2=nC_3H_7+HO_2$ | 3.98(13) | 0 | -24007 | 2.04(12) | 0 | 0 | [3] |
| 238. | $C_3H_8+O_2=iC_3H_7+HO_2$ | 3.98(13) | 0 | -24007 | 2.04(12) | 0 | 0 | [3] |
| 239. | $C_3H_8+H=nC_3H_7+H_2$ | 5.6(7) | 2 | -3892 | 9.1(12) | 0 | -7308 | [3] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------|---|----------|------|--------|----------|-------|---------|-----|
| 240. | $C_3H_8+H=iC_3H_7+H_2$ | 8.71(6) | 2 | -2527 | 7.76(12) | 0 | -8021 | [3] |
| 241. | $C_3H_8+O=nC_3H_7+OH$ | 1.12(14) | 0 | -3968 | 7.6(12) | 0 | -6196 | [3] |
| 242. | $C_3H_8+O=iC_3H_7+OH$ | 2.82(13) | 0 | -2628 | 1.86(12) | 0 | -4857 | [3] |
| 243. | $C_3H_8+OH=nC_3H_7+H_2O$ | 5.75(8) | 1.4 | -430 | 1.02(9) | 1.25 | -11306 | [3] |
| 244. | $C_3H_8+OH=iC_3H_7+H_2O$ | 4.79(8) | 1.4 | -430 | 8.51(8) | 1.25 | -11306 | [3] |
| 245. | $C_3H_8+HO_2=nC_3H_7+H_2O_2$ | 1.12(13) | 0 | -9805 | 2.34(12) | 0 | -4968 | [3] |
| 246. | $C_3H_8+HO_2=iC_3H_7+H_2O_2$ | 3.39(12) | 0 | -8592 | 6.92(11) | 0 | -3755 | [3] |
| 247. | $C_3H_8+CH_3=nC_3H_7+CH_4$ | 1.1(15) | 0 | -12706 | 4.37(15) | 0 | -16234 | [3] |
| 248. | $C_3H_8+CH_3=iC_3H_7+CH_4$ | 1.1(15) | 0 | -12706 | 4.37(15) | 0 | -16234 | [3] |
| 249. | $C_3H_8+CH_3O=nC_3H_7+CH_3OH$ | 3.02(11) | 0 | -3538 | 1.7(10) | 0 | -4887 | [3] |
| 250. | $C_3H_8+CH_3O=iC_3H_7+CH_3OH$ | 3.02(11) | 0 | -3538 | 1.7(10) | 0 | -4887 | [3] |
| 251. | $C_3H_8+C_2H_3=nC_3H_7+C_2H_4$ | 1(11) | 0 | -5256 | 1.32(11) | 0 | -8996 | [3] |
| 252. | $C_3H_8+C_2H_3=iC_3H_7+C_2H_4$ | 1(11) | 0 | -5256 | 1.32(11) | 0 | -8996 | [3] |
| 253. | $C_3H_8+C_2H_5=nC_3H_7+C_2H_6$ | 1(11) | 0 | -5256 | 3.63(10) | 0 | -5019 | [3] |
| 254. | $C_3H_8+C_2H_5=iC_3H_7+C_2H_6$ | 1(11) | 0 | -5256 | 3.63(10) | 0 | -5019 | [3] |
| 255. | $C_3H_8+C_3H_5=nC_3H_7+C_3H_6$ | 7.94(11) | 0 | -10361 | 1(11) | 0 | -4953 | [3] |
| 256. | $C_3H_8+C_3H_5=iC_3H_7+C_3H_6$ | 2(11) | 0 | -8137 | 3.98(10) | 0 | -4903 | [3] |
| 257. | $2nC_3H_7=C_3H_8+C_3H_6$ | 1.6(12) | 0 | 0 | 4.14(12) | 0.146 | -138989 | [8] |
| 258. | $2iC_3H_7=C_3H_8+C_3H_6$ | 2.4(12) | 0 | 0 | 5.59(10) | 0.236 | -119583 | [8] |
| 259. | $nC_3H_7=C_3H_6+H$ | 1.26(14) | 0 | -18700 | 1(13) | 0 | -758 | [3] |
| 260. | $iC_3H_7=C_3H_6+H$ | 6.31(13) | 0 | -18650 | 1(13) | 0 | -758 | [3] |
| 261. | $nC_3H_7=C_2H_4+CH_3$ | 9.55(13) | 0 | -15668 | 2.19(8) | 1 | -2926 | [3] |
| 262. | $iC_3H_7=C_2H_4+CH_3$ | 2(10) | 0 | -14910 | 4.57(4) | 1 | -2168 | [3] |
| 263. | $nC_3H_7+O_2=C_3H_6+HO_2$ | 1(12) | 0 | -2527 | 2(11) | 0 | -8835 | [3] |
| 264. | $iC_3H_7+O_2=C_3H_6+HO_2$ | 1(12) | 0 | -2527 | 2(11) | 0 | -8835 | [3] |
| 265. | $nC_3H_7+O_2=nC_3H_7O_2$ | 1(12) | 0 | 0 | 4.37(18) | -1 | -18710 | [5] |
| 266. | $iC_3H_7+O_2=iC_3H_7O_2$ | 1(12) | 0 | 0 | 4.37(18) | -1 | -18710 | [5] |
| 267. | $nC_3H_7+HO_2=nC_3H_7O+OH$ | 3.24(13) | 0 | 0 | 2(10) | 0 | 0 | [5] |
| 268. | $iC_3H_7+HO_2=iC_3H_7O+OH$ | 3.24(13) | 0 | 0 | 2(10) | 0 | 0 | [5] |
| 269. | $nC_3H_7+CH_3O_2=nC_3H_7O+CH_3O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 270. | $iC_3H_7+CH_3O_2=iC_3H_7O+CH_3O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 271. | $nC_3H_7+nC_3H_7O_2=2nC_3H_7O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 272. | $iC_3H_7+iC_3H_7O_2=2iC_3H_7O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 273. | $nC_3H_7+iC_3H_7O_2=nC_3H_7O+iC_3H_7O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 274. | $iC_3H_7+nC_3H_7O_2=iC_3H_7O+nC_3H_7O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 275. | $nC_3H_7O=C_2H_5+CH_2O$ | 1(15) | 0 | -10917 | 1(7) | 1 | -6874 | [5] |
| 276. | $iC_3H_7O=CH_3+CH_3CHO$ | 3.98(14) | 0 | -8693 | 1(7) | 1 | -6874 | [5] |
| 277. | $nC_3H_7O_2+HO_2=nC_3H_7O_2H+O_2$ | 4.57(10) | 0 | 1314 | 3.02(12) | 0 | -19711 | [5] |
| 278. | $iC_3H_7O_2+HO_2=iC_3H_7O_2H+O_2$ | 4.57(10) | 0 | 1314 | 3.02(12) | 0 | -19711 | [5] |
| 279. | $nC_3H_7O_2+CH_3=nC_3H_7O+CH_3O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 280. | $iC_3H_7O_2+CH_3=iC_3H_7O+CH_3O$ | 3.8(12) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 281. | $nC_3H_7O_2+CH_4=nC_3H_7O_2H+CH_3$ | 1.12(13) | 0 | -10341 | 7.6(11) | 0 | -647 | [5] |
| 282. | $iC_3H_7O_2+CH_4=iC_3H_7O_2H+CH_3$ | 1.12(13) | 0 | -10341 | 7.6(11) | 0 | -647 | [5] |
| 283. | $nC_3H_7O_2+CH_2O=nC_3H_7O_2H+HCO$ | 1.29(11) | 0 | -4549 | 2.51(10) | 0 | -5105 | [5] |
| 284. | $iC_3H_7O_2+CH_2O=iC_3H_7O_2H+HCO$ | 1.29(11) | 0 | -4549 | 2.51(10) | 0 | -5105 | [5] |
| 285. | $nC_3H_7O_2+CH_3OH=nC_3H_7O_2H+CH_2OH$ | 6.31(12) | 0 | -9785 | 1(9) | 0 | -5054 | [5] |
| 286. | $iC_3H_7O_2+CH_3OH=iC_3H_7O_2H+CH_2OH$ | 6.31(12) | 0 | -9785 | 1(9) | 0 | -5054 | [5] |
| 287. | $nC_3H_7O_2+C_2H_4=nC_3H_7O_2H+C_2H_3$ | 7.08(11) | 0 | -8648 | 2(10) | 0 | -7581 | [5] |
| 288. | $iC_3H_7O_2+C_2H_4=iC_3H_7O_2H+C_2H_3$ | 7.08(11) | 0 | -8648 | 2(10) | 0 | -7581 | [5] |
| 289. | $nC_3H_7O_2+CH_3CHO=nC_3H_7O_2H+CH_3CO$ | 1.15(11) | 0 | -5054 | 2.51(10) | 0 | -5105 | [5] |
| 290. | $iC_3H_7O_2+CH_3CHO=iC_3H_7O_2H+CH_3CO$ | 1.15(11) | 0 | -5054 | 2.51(10) | 0 | -5105 | [5] |
| 291. | $nC_3H_7O_2+C_3H_6=nC_3H_7O_2H+C_3H_5$ | 3.24(11) | 0 | -7531 | 2(10) | 0 | -7581 | [5] |
| 292. | $iC_3H_7O_2+C_3H_6=iC_3H_7O_2H+C_3H_5$ | 3.24(11) | 0 | -7531 | 2(10) | 0 | -7581 | [5] |
| 293. | $nC_3H_7O_2H=nC_3H_7O+OH$ | 3.98(15) | 0 | -21733 | 1(11) | 0 | 0 | [5] |
| 294. | $iC_3H_7O_2H=iC_3H_7O+OH$ | 3.98(15) | 0 | -21733 | 1(11) | 0 | 0 | [5] |
| 295. | $C_3H_6=C_2H_3+CH_3$ | 6.31(15) | 0 | -43365 | 1(10) | 1 | 0 | [3] |
| 296. | $C_3H_6=C_3H_5+H$ | 1(13) | 0 | -39422 | 1(11) | 0 | 0 | [3] |
| 297. | $C_3H_6+O_2=C_3H_5+HO_2$ | 1(14) | 0 | -19711 | 1(11) | 0 | 0 | [3] |
| 298. | $C_3H_6+H=C_3H_5+H_2$ | 5.01(12) | 0 | -756 | 1.51(12) | 0 | -8921 | [3] |
| 299. | $C_3H_6+O=C_2H_4+CH_2O$ | 6.76(4) | 2.56 | 570 | 6.61(4) | 2.56 | -40592 | [3] |
| 300. | $C_3H_6+O=C_2H_5+HCO$ | 6.76(4) | 2.56 | 570 | 1.35(4) | 2.56 | -14515 | [3] |
| 301. | $C_3H_6+O=CH_3CO+CH_3$ | 6.76(4) | 2.56 | 570 | 1.02(4) | 2.56 | -18518 | [3] |
| 302. | $C_3H_6+OH=C_3H_5+H_2O$ | 1(13) | 0 | -1547 | 3.8(7) | 0 | -36769 | [3] |
| 303. | $C_3H_6+OH=C_2H_5+CH_2O$ | 1(12) | 0 | 0 | 5.75(12) | 0 | -8744 | [3] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------------------------|--|----------|------|--------|-----------|------|--------|-----|
| 304. | $C_3H_6+OH=CH_3CHO+CH_3$ | 1(12) | 0 | 0 | 3.16(11) | 0 | -10310 | [3] |
| 305. | $C_3H_6+HO_2=C_3H_5+H_2O_2$ | 3.24(11) | 0 | -7531 | 3.39(10) | 0 | -7414 | [5] |
| 306. | $C_3H_6+HO_2=C_3H_6O+OH$ | 1.29(12) | 0 | -7531 | 0 | 0 | 0 | [5] |
| 307. | $C_3H_6+CH_3=C_3H_5+CH_4$ | 1.58(12) | 0 | -4448 | 1.32(13) | 0 | -12878 | [3] |
| 308. | $C_3H_6+HCO=C_3H_5+CH_2O$ | 1(13) | 0 | -14112 | 7.94(10) | 0 | -6250 | [5] |
| 309. | $C_3H_6+CH_3O=C_3H_5+CH_3OH$ | 1.35(11) | 0 | -2016 | 6.76(9) | 0 | -4536 | [5] |
| 310. | $C_3H_6+CH_3O_2=C_3H_5+CH_3O_2H$ | 3.24(11) | 0 | -7510 | 2(10) | 0 | -7560 | [5] |
| 311. | $C_3H_6+CH_3O_2=C_3H_6O+CH_3O$ | 1.05(11) | 0 | -7177 | 0 | 0 | 0 | [5] |
| 312. | $C_3H_6+C_2H_3=C_3H_5+C_2H_4$ | 3.02(12) | 0 | -7308 | 7.94(10) | 0 | -6250 | [5] |
| 313. | $C_3H_6+C_2H_4=C_3H_5+C_2H_5$ | 1(10) | 0 | -25200 | 1.26(12) | 0 | 0 | [5] |
| 314. | $C_3H_6+C_2H_5=C_3H_5+C_2H_6$ | 1(11) | 0 | -4939 | 7.94(11) | 0 | -10332 | [5] |
| 315. | $C_3H_6+C_2H_5O_2=C_3H_5+C_2H_5O_2H$ | 3.24(11) | 0 | -7531 | 2(10) | 0 | -7581 | [5] |
| 316. | $C_3H_6+C_3H_5O_2=C_3H_5+C_3H_5O_2H$ | 3.24(11) | 0 | -7531 | 2.57(10) | 0 | -7581 | [5] |
| 317. | $C_3H_6+C_3H_5O_2=C_3H_6O+C_3H_5O$ | 1.05(11) | 0 | -7177 | 0 | 0 | 0 | [5] |
| 318. | $CH_3CHO+C_3H_5=CH_3CO+C_3H_6$ | 7.94(10) | 0 | -6250 | 1(13) | 0 | -14112 | [5] |
| 319. | $C_3H_6+CH_3CO_3=C_3H_5+CH_3CO_3H$ | 3.24(11) | 0 | -7531 | 3.02(10) | 0 | -7430 | [5] |
| 320. | $C_3H_6O+H=C_3H_5O+H_2$ | 5.01(12) | 0 | -758 | 1(12) | 0 | -10108 | [5] |
| 321. | $C_3H_6O+O=C_3H_5O+OH$ | 3.02(13) | 0 | -2628 | 2(12) | 0 | -5054 | [5] |
| 322. | $C_3H_6O+OH=C_3H_5O+H_2O$ | 2(13) | 0 | -1546 | 3.98(7) | 0 | -36390 | [5] |
| 323. | $C_3H_6O+HO_2=C_3H_5O+H_2O_2$ | 3.24(11) | 0 | -7531 | 1(11) | 0 | -7581 | [5] |
| 324. | $C_3H_6O+CH_3=C_3H_5O+CH_4$ | 1.58(12) | 0 | -4448 | 7.08(12) | 0 | -12635 | [5] |
| 325. | $C_3H_6O+CH_3O=C_3H_5O+CH_3OH$ | 1.15(11) | 0 | -950 | 1(10) | 0 | -7581 | [5] |
| 326. | $C_3H_6O+CH_3O_2=C_3H_5O+CH_3O_2H$ | 1.58(11) | 0 | -6065 | 2(10) | 0 | -5560 | [5] |
| 327. | $C_3H_6O+C_2H_3=C_3H_5O+C_2H_4$ | 3.02(12) | 0 | -7329 | 1(11) | 0 | -7581 | [5] |
| 328. | $C_3H_6O+C_3H_5=C_3H_5O+C_3H_6$ | 7.94(10) | 0 | -6267 | 1(11) | 0 | -7581 | [5] |
| 329. | $C_3H_6O+C_3H_5O_2=C_3H_5O+C_3H_5O_2H$ | 1.58(11) | 0 | -6065 | 5.25(9) | 0 | -5560 | [5] |
| 330. | $C_3H_5=C_3H_4+H$ | 3.98(13) | 0 | -35379 | 1(8) | 1 | 0 | [3] |
| 331. | $C_3H_5+O_2=C_3H_4+HO_2$ | 6.03(11) | 0 | -5040 | 1.2(11) | 0 | -5040 | [3] |
| 332. | $C_3H_5+O_2=C_3H_5O_2$ | 1.2(10) | 0 | 1162 | 3.47(14) | -1 | -8036 | [5] |
| 333. | $C_3H_5+H=C_3H_4+H_2$ | 1(13) | 0 | 0 | 1(13) | 0 | -20160 | [3] |
| 334. | $C_2H_3+CH_3=C_3H_5+H$ | (**) | | | 1.68(14) | 0 | 0 | [2] |
| 335. | $C_3H_5+O=CH_2O+C_2H_3$ | 1.8(13) | 0 | 0 | 0 | 0 | 0 | [7] |
| 336. | $C_3H_5+OH=C_3H_4+H_2O$ | 6.02(12) | 0 | 0 | 0 | 0 | 0 | [7] |
| 337. | $C_3H_5+HO_2=C_3H_5O+OH$ | 8.91(12) | 0 | 0 | 2(10) | 0 | 0 | [5] |
| 338. | $C_3H_5+CH_3=C_3H_4+CH_4$ | 1(12) | 0 | 0 | 1(13) | 0 | -20160 | [3] |
| 339. | $C_3H_5+CH_3O_2=C_3H_5O+CH_3O$ | 3.8(11) | 0 | 606 | 3(10) | 0 | 0 | [5] |
| 340. | $C_3H_5O=CH_2O+C_2H_3$ | 1(14) | 0 | -10917 | 1(11) | 0 | -4549 | [5] |
| 341. | $C_3H_5O_2+HO_2=C_3H_5O_2H+O_2$ | 4.57(10) | 0 | 1314 | 3.02(12) | 0 | -19711 | [5] |
| 342. | $C_3H_5O_2+HO_2=C_3H_5O+OH+O_2$ | 1(12) | 0 | 0 | 0 | 0 | 0 | [5] |
| 343. | $C_3H_5O_2+CH_3=C_3H_5O+CH_3O$ | 3.8(11) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 344. | $C_3H_5O_2+CH_4=C_3H_5O_2H+CH_3$ | 1.12(13) | 0 | -10341 | 7.6(11) | 0 | -647 | [5] |
| 345. | $C_3H_5O_2+CH_2O=C_3H_5O_2H+HCO$ | 1.29(11) | 0 | -5307 | 2.51(10) | 0 | -5107 | [5] |
| 346. | $C_3H_5O_2+CH_3O_2=C_3H_5O+CH_3O+O_2$ | 3.72(12) | 0 | -1112 | 0 | 0 | 0 | [5] |
| 347. | $C_3H_5O_2+CH_3CHO=C_3H_5O_2H+CH_3CO$ | 1.15(11) | 0 | -5054 | 2.51(10) | 0 | -5107 | [5] |
| 348. | $C_3H_5O_2+C_3H_5=2C_3H_5O$ | 3.8(11) | 0 | 606 | 2(10) | 0 | 0 | [5] |
| 349. | $2C_3H_5O_2=2C_3H_5O+O_2$ | 3.72(12) | 0 | -1112 | 0 | 0 | 0 | [5] |
| 350. | $C_3H_5O_2H=C_3H_5O+OH$ | 3.98(15) | 0 | -21733 | 1(11) | 0 | 0 | [5] |
| 351. | $C_3H_4+O=HCO+C_2H_3$ | 1(12) | 0 | 0 | 2.95(10) | 0 | -15533 | [3] |
| 352. | $C_3H_4+O=CH_2O+C_2H_2$ | 1(12) | 0 | 0 | 1.07(12) | 0 | -41308 | [3] |
| 353. | $C_3H_4+OH=HCO+C_2H_4$ | 1(12) | 0 | 0 | 5.9(11) | 0 | -17040 | [3] |
| 354. | $C_3H_4+OH=CH_2O+C_2H_3$ | 1(12) | 0 | 0 | 8.51(11) | 0 | -9193 | [3] |
| Reactions with C_4H_9 | | | | | | | | |
| 355. | $nC_4H_{10}=2C_2H_5$ | 2(16) | 0 | -40915 | 1(13) | 0 | 0 | [8] |
| 356. | $nC_4H_{10}=nC_3H_7+CH_3$ | 2(16) | 0 | -40915 | 2.06(7) | 1.84 | 3923 | [8] |
| 357. | $nC_4H_{10}+O_2=nC_4H_9+HO_2$ | 2.51(13) | 0 | -24669 | 3.81(-12) | 6.85 | 4308 | [8] |
| 358. | $nC_4H_{10}+O_2=sC_4H_9+HO_2$ | 3.98(13) | 0 | -23947 | 3.57(-12) | 6.98 | 3261 | [8] |
| 359. | $nC_4H_{10}+H=nC_4H_9+H_2$ | 4.4(11) | 0 | 0 | 4.01(-9) | 6.27 | -3971 | [8] |
| 360. | $nC_4H_{10}+H=sC_4H_9+H_2$ | 4.4(11) | 0 | 0 | 3.65(-9) | 6.4 | -5054 | [8] |
| 361. | $nC_4H_{10}+O=nC_4H_9+OH$ | 3(13) | 0 | -2888 | 5.12(-10) | 6.25 | -1094 | [8] |
| 362. | $nC_4H_{10}+O=sC_4H_9+OH$ | 5.2(13) | 0 | -2238 | 5.24(-10) | 6.37 | -2178 | [8] |
| 363. | $nC_4H_{10}+OH=nC_4H_9+H_2O$ | 4.13(7) | 1.73 | -379 | 2.01(-14) | 7.85 | -7256 | [8] |
| 364. | $nC_4H_{10}+OH=sC_4H_9+H_2O$ | 7.22(7) | 1.64 | 124 | 2.97(-14) | 7.88 | -8484 | [8] |
| 365. | $nC_4H_{10}+HO_2=nC_4H_9+H_2O_2$ | 1.68(13) | 0 | -10289 | 3(-7) | 5.58 | -1360 | [8] |
| 366. | $nC_4H_{10}+HO_2=sC_4H_9+H_2O_2$ | 1.12(13) | 0 | -8905 | 1.18(-7) | 5.7 | -1709 | [8] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|----------|------|---------|-----------|-------|--------|-----|
| 367. | $nC_4H_{10}+CH_3=nC_4H_9+CH_4$ | 1.29(12) | 0 | -5836 | 1(13) | 0 | -9350 | [8] |
| 368. | $nC_4H_{10}+CH_3=sC_4H_9+CH_4$ | 7.94(11) | 0 | -4777 | 6.31(12) | 0 | -8291 | [8] |
| 369. | $nC_4H_{10}+CH_3O=nC_4H_9+CH_3OH$ | 3.16(10) | 0 | -1456 | 1.24(-11) | 6.02 | -682 | [8] |
| 370. | $nC_4H_{10}+CH_3O=sC_4H_9+CH_3OH$ | 3.16(10) | 0 | -1456 | 7.33(-12) | 6.15 | -2419 | [8] |
| 371. | $nC_4H_{10}+CH_3O_2=nC_4H_9+CH_3O_2H$ | 1.68(13) | 0 | -10289 | 6.13(-19) | 8.97 | 613 | [8] |
| 372. | $nC_4H_{10}+CH_3O_2=sC_4H_9+CH_3O_2H$ | 1.12(13) | 0 | -8905 | 2.42(-19) | 9.1 | 262 | [8] |
| 373. | $nC_4H_{10}+CH_3CO_3=nC_4H_9+CH_3CO_3H$ | 1.68(13) | 0 | -10289 | 1.26(-11) | 6.76 | -800 | [8] |
| 374. | $nC_4H_{10}+CH_3CO_3=sC_4H_9+CH_3CO_3H$ | 1.12(13) | 0 | -8905 | 4.97(-12) | 6.89 | -1149 | [8] |
| 375. | $nC_4H_{10}+C_2H_5O_2=nC_4H_9+C_2H_5O_2H$ | 1.68(13) | 0 | -10289 | 1.13(-12) | 6.76 | 2178 | [8] |
| 376. | $nC_4H_{10}+C_2H_5O_2=sC_4H_9+C_2H_5O_2H$ | 1.12(13) | 0 | -8905 | 4.44(-13) | 6.89 | 1829 | [8] |
| 377. | $nC_4H_{10}+nC_3H_7O_2=nC_4H_9+nC_3H_7O_2H$ | 1.68(13) | 0 | -10289 | 1.13(-12) | 6.76 | 2178 | [8] |
| 378. | $nC_4H_{10}+nC_3H_7O_2=sC_4H_9+nC_3H_7O_2H$ | 1.12(13) | 0 | -8905 | 4.45(-13) | 6.89 | 1829 | [8] |
| 379. | $nC_4H_{10}+iC_3H_7O_2=nC_4H_9+iC_3H_7O_2H$ | 1.68(13) | 0 | -10289 | 1.4(-12) | 6.73 | 2166 | [8] |
| 380. | $nC_4H_{10}+iC_3H_7O_2=sC_4H_9+iC_3H_7O_2H$ | 1.12(13) | 0 | -8905 | 5.5(-13) | 6.86 | 1817 | [8] |
| 381. | $nC_4H_9=C_2H_5+C_2H_4$ | 3.7(13) | 0 | -14440 | 8.92(22) | -3.35 | -6522 | [8] |
| 382. | $sC_4H_9=C_3H_6+CH_3$ | 2.3(14) | 0 | -16486 | 7.84(25) | -3.9 | -5704 | [8] |
| 383. | $sC_4H_9=C_4H_8+H$ | 8.3(13) | 0 | -19200 | 0 | 0 | 0 | [7] |
| 384. | $nC_4H_9+O_2=C_4H_8+HO_2$ | 1.12(10) | 0 | 758 | 1.95(11) | 0 | -7978 | [8] |
| 385. | $sC_4H_9+O_2=C_4H_8+HO_2$ | 1.12(10) | 0 | 758 | 1.95(11) | 0 | -9242 | [8] |
| 386. | $C_4H_8=C_2H_3+C_2H_5$ | 0 | 0 | 0 | (**) | | | [2] |
| 387. | $C_4H_8+O=CH_2O+C_3H_6$ | 5(12) | 0 | 0 | 0 | 0 | 0 | [4] |
| 388. | $C_4H_8+OH=CH_2O+nC_3H_7$ | 1.5(12) | 0 | 0 | 0 | 0 | 0 | [4] |
| 389. | $C_4H_6=2C_2H_3$ | 4(19) | -1 | -49468 | (**) | | | [4] |
| 390. | $C_4H_6+O=C_3H_4+CH_2O$ | 1(12) | 0 | 0 | 0 | 0 | 0 | [4] |
| 391. | $C_4H_6+H=C_2H_3+C_2H_4$ | 1(13) | 0 | -2369 | 5(11) | 0 | -3676 | [4] |
| 392. | $C_4H_6+OH=C_3H_5+CH_2O$ | 1(12) | 0 | 0 | 0 | 0 | 0 | [4] |
| 393. | $C_4H_6+OH=C_2H_3+CH_3CHO$ | 1(12) | 0 | 0 | 0 | 0 | 0 | [4] |
| Reactions with O ₃ | | | | | | | | |
| 394. | $O_3+M=O_2+O+M$ | 4(14) | 0 | -11400 | 6.9(12) | 0 | 1050 | [1] |
| 395. | $H+O_3=OH+O_2$ | 2.3(11) | 0.75 | 0 | 4.4(7) | 1.44 | -38600 | [1] |
| 396. | $O_3+O=2O_2$ | 1.1(13) | 0 | -2300 | 1.2(13) | 0 | -50500 | [1] |
| 397. | $O_3+OH=HO_2+O_2$ | 9.6(11) | 0 | -1000 | 9(8) | 0 | 0 | [1] |
| 398. | $O_3+HO_2=OH+2O_2$ | 2(10) | 0 | -1000 | | | | [1] |
| 399. | $O_3+H_2=OH+HO_2$ | 6.02(10) | 0 | -10000 | | | | [1] |
| Reactions with N, N ₂ , NO | | | | | | | | |
| 400. | $NO+M=N+O+M$ | 5.25(17) | -0.5 | -75600 | 1(17) | -0.5 | 0 | [1] |
| 401. | $N_2+M=2N+M$ | 3.72(21) | -1.6 | -113272 | 7.94(19) | -1.6 | 0 | [1] |
| 402. | $O+N_2=N+NO$ | 1.74(14) | 0 | -38455 | 4(13) | 0 | -504 | [1] |
| 403. | $O+N\dot{O}=N+O_2$ | 1.51(9) | 1 | -19439 | 6.46(9) | 1 | -3147 | [1] |
| 404. | $H+NO=N+OH$ | 1.7(14) | 0 | -24500 | 4.5(13) | 0 | 0 | [1] |
| 405. | $N+HO_2=NO+OH$ | 1(13) | 0 | -1000 | 2.69(12) | 0 | -41630 | [1] |
| Reactions with NO ₂ | | | | | | | | |
| 406. | $OH+NO_2=NO+HO_2$ | 1(11) | 0.5 | -6000 | 3(12) | 0.5 | -1200 | [1] |
| 407. | $OH+NO=H+NO_2$ | 2(11) | 0.5 | -15500 | 3.5(14) | 0 | -740 | [1] |
| 408. | $O_2+NO=O+NO_2$ | 1(12) | 0 | -23568 | 1(13) | 0 | -302 | [1] |
| 409. | $N\dot{O}_2+M=N+O+M$ | 1.1(16) | 0 | -32712 | 1.1(15) | 0 | 941 | [1] |
| 410. | $NO_2+N=2NO$ | 3.6(12) | 0 | 0 | 1.1(11) | 0 | -39200 | [1] |
| 411. | $2N\dot{O}_2=2NO+O_2$ | 2(12) | 0 | -13500 | 1.2(9) | 0 | 530 | [1] |
| 412. | $O_3+N\dot{O}=NO_2+O_2$ | 1.2(12) | 0 | -1400 | | | | [1] |
| Reactions with HNO ₂ | | | | | | | | |
| 413. | $HNO_2+M=NO+OH+M$ | 5(17) | -1 | -25000 | 8(15) | 0 | 1000 | [1] |
| 414. | $H_2+N\dot{O}_2=H+HNO_2$ | 2.4(13) | 0 | -14500 | 5(11) | 0.5 | -1500 | [1] |
| 415. | $O+HNO_2=OH+NO_2$ | 6.02(11) | 0 | -2000 | | | | [1] |
| 416. | $OH+HNO_2=H_2O+N\dot{O}_2$ | 1.52(12) | 0 | 28 | 8.31(12) | 0 | -21136 | [1] |
| Reactions with HNO, HNO ₃ , HNO ₄ | | | | | | | | |
| 417. | $O+HNO_2=O_2+HNO$ | 3.01(12) | 0 | -8000 | | | | [1] |
| 418. | $HNO+O=NO+OH$ | 5.01(11) | 0.5 | -1000 | | | | [1] |
| 419. | $HNO+OH=NO+H_2O$ | 1.26(12) | 0.5 | -1000 | | | | [1] |
| 420. | $NO+HO_2=HNO+O_2$ | 2(11) | 0 | -1000 | | | | [1] |
| 421. | $HNO+H\dot{O}_2=NO+H_2O_2$ | 3.16(11) | 0.5 | -1000 | | | | [1] |
| 422. | $HNO+H=N\dot{O}+H_2$ | 1.26(13) | 0 | -2000 | | | | [1] |
| 423. | $HNO+M=H+NO+M$ | 2(16) | 0 | -24500 | | | | [1] |
| 424. | $HNO_3+O=O_2+HNO_2$ | 6(12) | 0 | -8000 | | | | [1] |
| 425. | $HNO_3+M=OH+NO_2+M$ | 1.6(15) | 0 | -15400 | 2.4(16) | 0 | 1016 | [1] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|----------|------|--------|---------|---|--------|-----|
| 426. | $\text{HNO}_3 + \text{OH} = \text{NO}_3 + \text{H}_2\text{O}$ | 1.93(9) | 2.34 | -1014 | | | | [1] |
| 427. | $\text{HNO}_4 + \text{OH} = \text{H}_2\text{O} + \text{NO}_2 + \text{O}_2$ | 7.8(11) | 0 | 380 | | | | [1] |
| Reactions with N_2O , NO_3 | | | | | | | | |
| 428. | $\text{N}_2\text{O} + \text{M} = \text{N}_2 + \text{O} + \text{M}$ | 3.98(20) | -1.5 | -75490 | 1.4(13) | 0 | -10400 | [1] |
| 429. | $\text{N}_2\text{O} + \text{O} = 2\text{NO}$ | 6.92(13) | 0 | -13400 | 1.3(12) | 0 | -32100 | [1] |
| 430. | $\text{N}_2\text{O} + \text{O} = \text{N}_2 + \text{O}_2$ | 1(14) | 0 | -14100 | 1.3(12) | 0 | -32100 | [1] |
| 431. | $\text{NO}_2 + \text{N} = \text{N}_2\text{O} + \text{O}$ | 5.01(12) | 0 | 0 | | | | [1] |
| 432. | $\text{NO} + \text{N}_2\text{O} = \text{N}_2 + \text{NO}_2$ | 1(14) | 0 | -25000 | | | | [1] |
| 433. | $\text{N}_2\text{O} + \text{N} = \text{N}_2 + \text{NO}$ | 1(13) | 0 | -10000 | | | | [1] |
| 434. | $\text{N}_2\text{O} + \text{OH} = \text{N}_2 + \text{HO}_2$ | 6.31(11) | 0 | -5000 | | | | [1] |
| 435. | $\text{N}_2\text{O} + \text{H} = \text{N}_2 + \text{OH}$ | 7.59(13) | 0 | -7600 | | | | [1] |
| 436. | $\text{O}_3 + \text{NO}_2 = \text{NO}_3 + \text{O}_2$ | 7.22(10) | 0 | -2450 | | | | [1] |
| 437. | $\text{O}_3 + \text{N}_2 = \text{N}_2\text{O} + \text{O}_2$ | 6(10) | 0 | -10000 | | | | [1] |
| 438. | $\text{HNO}_3 + \text{M} = \text{H} + \text{NO}_3 + \text{M}$ | 1.6(15) | 0 | -15400 | | | | [1] |
| 439. | $\text{HNO}_3 + \text{O} = \text{OH} + \text{NO}_3$ | 6(11) | 0 | -4000 | | | | [1] |
| 440. | $\text{NO}_3 + \text{M} = \text{NO}_2 + \text{O} + \text{M}$ | 1.08(16) | 0 | -32000 | | | | [1] |
| 441. | $\text{NO}_3 + \text{H} = \text{NO}_2 + \text{OH}$ | 3.5(14) | 0 | -750 | | | | [1] |
| Reactions with N_xH_y | | | | | | | | |
| 442. | $\text{N}_2\text{H}_4 + \text{M} = 2\text{NH}_2 + \text{M}$ | 3.98(15) | 0 | -20600 | | | | [1] |
| 443. | $\text{N}_2\text{H}_4 + \text{M} = \text{N}_2\text{H}_3 + \text{H} + \text{M}$ | 1(15) | 0 | -32000 | | | | [1] |
| 444. | $\text{N}_2\text{H}_3 + \text{M} = \text{N}_2\text{H}_2 + \text{H} + \text{M}$ | 1(16) | 0 | -25000 | | | | [1] |
| 445. | $\text{N}_2\text{H}_3 + \text{M} = \text{NH}_2 + \text{NH} + \text{M}$ | 1(16) | 0 | -21000 | | | | [1] |
| 446. | $\text{N}_2\text{H}_2 + \text{M} = \text{N}_2\text{H} + \text{H} + \text{M}$ | 1(16) | 0 | -25000 | | | | [1] |
| 447. | $\text{N}_2\text{H}_2 + \text{M} = 2\text{NH} + \text{M}$ | 3.16(16) | 0 | -50000 | | | | [1] |
| 448. | $\text{N}_2\text{H} + \text{M} = \text{N}_2 + \text{H} + \text{M}$ | 2(14) | 0 | -10000 | | | | [1] |
| 449. | $\text{N}_2\text{H} + \text{M} = \text{NH} + \text{N} + \text{M}$ | 1(15) | 0 | -35000 | | | | [1] |
| 450. | $\text{NH}_3 + \text{M} = \text{NH}_2 + \text{H} + \text{M}$ | 2.51(16) | 0 | -47200 | | | | [1] |
| 451. | $\text{NH}_3 + \text{M} = \text{NH} + \text{H}_2 + \text{M}$ | 6.31(14) | 0 | -47000 | | | | [1] |
| 452. | $\text{NH}_2 + \text{M} = \text{NH} + \text{H} + \text{M}$ | 3.16(23) | -2 | -46000 | | | | [1] |
| 453. | $\text{NH} + \text{M} = \text{N} + \text{H} + \text{M}$ | 3.16(21) | -2 | -42000 | | | | [1] |
| 454. | $\text{N}_2\text{H}_4 + \text{H} = \text{N}_2\text{H}_3 + \text{H}_2$ | 1.29(13) | 0 | -1260 | | | | [1] |
| 455. | $\text{N}_2\text{H}_4 + \text{H} = \text{NH}_2 + \text{NH}_3$ | 1.12(9) | 0 | -1560 | | | | [1] |
| 456. | $\text{N}_2\text{H}_3 + \text{H} = \text{N}_2\text{H}_2 + \text{H}_2$ | 1(12) | 0 | -1000 | | | | [1] |
| 457. | $\text{N}_2\text{H}_3 + \text{H} = 2\text{NH}_2$ | 1.58(12) | 0 | 0 | | | | [1] |
| 458. | $\text{N}_2\text{H}_3 + \text{H} = \text{NH} + \text{NH}_3$ | 1(11) | 0 | 0 | | | | [1] |
| 459. | $\text{N}_2\text{H}_2 + \text{H} = \text{N}_2\text{H} + \text{H}_2$ | 1(13) | 0 | -500 | | | | [1] |
| 460. | $\text{N}_2\text{H} + \text{H} = \text{N}_2 + \text{H}_2$ | 3.98(13) | 0 | -1500 | | | | [1] |
| 461. | $\text{NH}_3 + \text{H} = \text{NH}_2 + \text{H}_2$ | 1.26(14) | 0 | -10820 | | | | [1] |
| 462. | $\text{NH}_2 + \text{H} = \text{NH} + \text{H}_2$ | 2(13) | 0 | 0 | | | | [1] |
| 463. | $\text{NH} + \text{H} = \text{N} + \text{H}_2$ | 5.01(13) | 0 | -1000 | | | | [1] |
| 464. | $\text{N}_2\text{H}_4 + \text{NH} = \text{NH}_2 + \text{N}_2\text{H}_3$ | 1(12) | 0.5 | -1000 | | | | [1] |
| 465. | $\text{N}_2\text{H}_2 + \text{NH} = \text{N}_2\text{H} + \text{NH}_2$ | 1(13) | 0 | -500 | | | | [1] |
| 466. | $\text{N}_2\text{H} + \text{NH} = \text{N}_2 + \text{NH}_2$ | 2(11) | 0.5 | -1000 | | | | [1] |
| 467. | $2\text{NH} = \text{NH}_2 + \text{N}$ | 2(11) | 0.5 | -1000 | | | | [1] |
| 468. | $2\text{NH} = \text{N}_2\text{H} + \text{H}$ | 7.94(11) | 0.5 | -500 | | | | [1] |
| 469. | $\text{N}_2\text{H}_4 + \text{NH}_2 = \text{N}_2\text{H}_3 + \text{NH}_3$ | 3.98(11) | 0.5 | -1000 | | | | [1] |
| 470. | $\text{N}_2\text{H}_3 + \text{NH}_2 = \text{N}_2\text{H}_2 + \text{NH}_3$ | 1(11) | 0.5 | 0 | | | | [1] |
| 471. | $\text{N}_2\text{H}_2 + \text{NH}_2 = \text{N}_2\text{H} + \text{NH}_3$ | 1(13) | 0 | -2000 | | | | [1] |
| 472. | $\text{N}_2\text{H}_2 + \text{NH}_2 = \text{NH} + \text{N}_2\text{H}_3$ | 1(11) | 0.5 | -17000 | | | | [1] |
| 473. | $\text{N}_2\text{H} + \text{NH}_2 = \text{N}_2 + \text{NH}_3$ | 1(13) | 0 | 0 | | | | [1] |
| 474. | $\text{NH}_3 + \text{NH}_2 = \text{N}_2\text{H}_3 + \text{H}_2$ | 7.94(11) | 0.5 | -10850 | | | | [1] |
| 475. | $2\text{NH}_2 = \text{NH}_3 + \text{NH}$ | 6.31(12) | 0 | -5000 | | | | [1] |
| 476. | $2\text{NH}_2 = \text{N}_2\text{H}_2 + \text{H}_2$ | 3.98(13) | 0 | -6000 | | | | [1] |
| 477. | $\text{NH}_2 + \text{NH} = \text{N}_2\text{H}_2 + \text{H}$ | 3.16(13) | 0 | -500 | | | | [1] |
| 478. | $\text{N}_2\text{H}_4 + \text{N}_2\text{H}_2 = 2\text{N}_2\text{H}_3$ | 2.51(10) | 0.5 | -15000 | | | | [1] |
| 479. | $\text{N}_2\text{H}_3 + \text{N}_2\text{H}_2 = \text{N}_2\text{H}_4 + \text{N}_2\text{H}$ | 1(13) | 0 | -5000 | | | | [1] |
| 480. | $2\text{N}_2\text{H}_2 = \text{N}_2\text{H} + \text{N}_2\text{H}_3$ | 1(13) | 0 | -5000 | | | | [1] |
| 481. | $2\text{N}_2\text{H} = \text{N}_2\text{H}_2 + \text{N}_2$ | 1(13) | 0 | -5000 | | | | [1] |
| 482. | $\text{NH} + \text{N} = \text{N}_2 + \text{H}$ | 6.31(11) | 0.5 | 0 | | | | [1] |
| 483. | $\text{N}_2\text{H} + \text{N} = \text{NH} + \text{N}_2$ | 3.16(13) | 0 | -1000 | | | | [1] |
| 484. | $\text{N}_2\text{H}_4 + \text{O} = \text{N}_2\text{H}_2 + \text{H}_2\text{O}$ | 6.31(13) | 0 | -600 | | | | [1] |
| 485. | $\text{N}_2\text{H}_4 + \text{O} = \text{N}_2\text{H}_3 + \text{OH}$ | 2.51(12) | 0 | -600 | | | | [1] |
| 486. | $\text{N}_2\text{H}_3 + \text{O} = \text{N}_2\text{H}_2 + \text{OH}$ | 3.16(11) | 0.5 | 0 | | | | [1] |
| 487. | $\text{N}_2\text{H}_3 + \text{O} = \text{N}_2\text{H} + \text{H}_2\text{O}$ | 3.16(11) | 0.5 | 0 | | | | [1] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|-----------------------------|----------|------|--------|----------|------|--------|-----|
| 488. | $N_2H_2+O=N_2H+OH$ | 1(11) | 0.5 | 0 | | | | [1] |
| 489. | $N_2H+O=N_2+OH$ | 1(13) | 0 | -2500 | | | | [1] |
| 490. | $N_2H+O=N_2O+H$ | 1(13) | 0 | -1500 | | | | [1] |
| 491. | $NH_3+O=NH_2+OH$ | 2(13) | 0 | -4470 | | | | [1] |
| 492. | $NH_2+O=NH+OH$ | 1.26(16) | -0.5 | 0 | | | | [1] |
| 493. | $NH_2+O=HNO+H$ | 6.31(14) | -0.5 | 0 | | | | [1] |
| 494. | $NH+O=N+OH$ | 6.31(11) | 0.5 | -4000 | | | | [1] |
| 495. | $NH+O=NO+H$ | 6.31(11) | 0.5 | 0 | | | | [1] |
| 496. | $N_2H_4+OH=N_2H_3+H_2O$ | 3.98(13) | 0 | 0 | | | | [1] |
| 497. | $N_2H_3+OH=N_2H_2+H_2O$ | 1(13) | 0 | -1000 | | | | [1] |
| 498. | $N_2H_2+OH=N_2H+H_2O$ | 1(13) | 0 | -1000 | | | | [1] |
| 499. | $N_2H+OH=N_2+H_2O$ | 3.16(13) | 0 | 0 | | | | [1] |
| 500. | $NH_3+OH=NH_2+H_2O$ | 5.75(13) | 0 | -4055 | | | | [1] |
| 501. | $NH_2+OH=NH+H_2O$ | 5.01(11) | 0.5 | -1000 | | | | [1] |
| 502. | $NH+OH=N+H_2O$ | 5.01(11) | 0.5 | -1000 | | | | [1] |
| 503. | $HNO+H=NH+OH$ | | | | 1(12) | 0.5 | -1008 | [1] |
| 504. | $N_2H_4+HO_2=N_2H_3+H_2O_2$ | 3.98(13) | 0 | -1000 | | | | [1] |
| 505. | $N_2H_3+HO_2=N_2H_2+H_2O_2$ | 1(13) | 0 | -1000 | | | | [1] |
| 506. | $N_2H_2+HO_2=N_2H+H_2O_2$ | 1(13) | 0 | -1000 | | | | [1] |
| 507. | $N_2H+HO_2=N_2+H_2O_2$ | 1(13) | 0 | -1000 | | | | [1] |
| 508. | $NH_3+HO_2=NH_2+H_2O_2$ | 2.51(12) | 0 | -12000 | | | | [1] |
| 509. | $NH_2+HO_2=NH_3+O_2$ | 1(13) | 0 | -1000 | | | | [6] |
| 510. | $NH_2+HO_2=NH+H_2O_2$ | 1(13) | 0 | -1000 | | | | [1] |
| 511. | $NH+HO_2=HNO+OH$ | 1(13) | 0 | -1000 | | | | [1] |
| 512. | $N+HO_2=NH+O_2$ | 1(13) | 0 | -1000 | | | | [1] |
| 513. | $HNO+N=NO+NH$ | 1(13) | 0 | -1000 | | | | [1] |
| 514. | $NO+NH=N_2O+H$ | 1(12) | 0 | -252 | | | | [1] |
| 515. | $NH_2+NO=N_2+H_2O$ | 6.31(19) | -2.5 | -958 | | | | [1] |
| 516. | $NH_2+NO=N_2+H+OH$ | 6.31(19) | -2.5 | -950 | | | | [1] |
| 517. | $NH_2+NO=N_2O+H_2$ | 5.01(13) | 0 | -12449 | | | | [1] |
| 518. | $NO_2+NH=HNO+NO$ | 1(11) | 0.5 | -2016 | | | | [1] |
| 519. | $NO_2+NH_2=N_2O+H_2O$ | 2(20) | -3 | 0 | | | | [6] |
| 520. | $N_2O+NH=N_2+HNO$ | 2(12) | 0 | -3000 | | | | [1] |
| 521. | $NH_2+O_2=HNO+OH$ | 2(12) | 0 | -7560 | | | | [1] |
| 522. | $NH_2+O_2=NH+HO_2$ | 1(14) | 0 | -25200 | | | | [1] |
| 523. | $NH+O_2=HNO+O$ | 1(12) | 0 | -1613 | | | | [1] |
| 524. | $N_2H+O_2=N_2+HO_2$ | 1(13) | 0 | -2016 | | | | [1] |
| Reactions with CN, C ₂ N ₂ , HCN, NCO, C ₂ N | | | | | | | | |
| 525. | $HCN+M=CN+H+M$ | 5.75(16) | 0 | -59018 | | | | [6] |
| 526. | $HCN+O=CN+OH$ | 5.01(13) | 0 | -11088 | 7.08(12) | 0 | -1008 | [6] |
| 527. | $HCN+O=NCO+H$ | 1.82(8) | 1.5 | -3734 | 5.01(8) | 1.5 | -3931 | [6] |
| 528. | $HCN+O=NH+CO$ | 2.19(13) | 0 | -7706 | 7.94(12) | 0 | -22680 | [6] |
| 529. | $HCN+OH=CN+H_2O$ | 4.37(12) | 0 | -4576 | 6.31(12) | 0 | -3034 | [6] |
| 530. | $HCN+OH=NH_2+CO$ | 7.8(-4) | 4 | -2016 | 6.6(-4) | 4 | -14061 | [6] |
| 531. | $HCN+CH=C_2N+H_2$ | 1(13) | 0 | 0 | 3.31(13) | 0 | -19832 | [6] |
| 532. | $CN+H_2=HCN+H$ | 2.51(2) | 3.62 | -963 | 7.76(2) | 3.62 | -10282 | [6] |
| 533. | $CN+O_2=NCO+O$ | 5.62(12) | 0 | 0 | 1.35(13) | 0 | -2722 | [6] |
| 534. | $CN+O=CO+N$ | 2(13) | 0 | -242 | 1.05(14) | 0 | -39110 | [6] |
| 535. | $CN+OH=NCO+H$ | 5.62(13) | 0 | 0 | 1.07(15) | 0 | -10292 | [6] |
| 536. | $CN+N=C+N_2$ | 1.05(15) | -0.5 | 0 | 6.31(13) | 0 | -23194 | [6] |
| 537. | $CN+NO_2=NCO+NO$ | 3.02(13) | 0 | 0 | 7.08(13) | 0 | -25770 | [6] |
| 538. | $CN+N_2O=NCO+N_2$ | 1(13) | 0 | 0 | 1.29(13) | 0 | -44042 | [6] |
| 539. | $CN+HCN=C_2N_2+H$ | 2(13) | 0 | 0 | 4.79(14) | 0 | -3457 | [6] |
| 540. | $CN+C=C_2+N$ | 5.01(13) | 0 | -13018 | 4.27(13) | 0 | 6703 | [6] |
| 541. | $CN+CN=C_2+N_2$ | 6.31(11) | 0 | 0 | 1.26(12) | 0 | -3397 | [6] |
| 542. | $CN+CH=C_2N+H$ | 1(13) | 0 | 0 | 1(14) | 0 | -28980 | [6] |
| 543. | $NCO+M=CO+N+M$ | 6.31(16) | -0.5 | -24081 | | | | [6] |
| 544. | $NCO+H=NH+CO$ | 3.98(13) | 0 | 0 | 5.01(12) | 0 | -14767 | [6] |
| 545. | $NCO+NO=N_2O+CO$ | 1(13) | 0 | 242 | 3.16(14) | 0 | -33768 | [6] |
| 546. | $NCO+O=NO+CO$ | 5.75(13) | 0 | 0 | | | | [6] |
| 547. | $NCO+N=N_2+CO$ | 2(13) | 0 | 0 | | | | [6] |
| 548. | $NCO+OH=NO+CO+H$ | 1(13) | 0 | 0 | | | | [6] |
| 549. | $NO+CH_3=HCN+H_2O$ | 4.27(12) | 0 | -10231 | | | | [6] |
| 550. | $NO+CH_2=HCN+OH$ | 1.41(12) | 0 | 605 | | | | [6] |

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------|--|----------|---|--------|----------|---|--------|-----|
| 551. | NO+CH=HCN+O | 1.2(14) | 0 | 0 | | | | [6] |
| 552. | NO+C=CN+O | 6.61(13) | 0 | 0 | 1.26(14) | 0 | -14818 | [6] |
| 553. | CH+N ₂ =HCN+N | 4.37(12) | 0 | -11088 | 2.19(13) | 0 | -8850 | [6] |
| 554. | CH ₂ +N ₂ =HCN+NH | 1(13) | 0 | -37649 | 7.24(12) | 0 | -22116 | [6] |
| 555. | CH ₃ +N=HCN+H+H | 7.08(13) | 0 | 0 | | | | [6] |
| 556. | CH ₂ +N=HCN+H | 5.01(12) | 0 | 0 | | | | [6] |
| 557. | CH+N=CN+H | 1.29(13) | 0 | 0 | | | | [6] |
| 558. | N+CO ₂ =NO+CO | 1.9(11) | 0 | -1714 | | | | [6] |
| 559. | N+C ₂ HO=HCN+CO | 5.01(13) | 0 | 0 | | | | [6] |
| 560. | N+C ₂ H ₃ =HCN+CH ₂ | 2(13) | 0 | 0 | 3.98(12) | 0 | -25427 | [6] |
| 561. | N+C ₃ H ₃ =HCN+C ₂ H ₂ | 1(13) | 0 | 0 | | | | [6] |
| 562. | C ₂ N ₂ +O=NCO+CN | 4.57(12) | 0 | -4476 | 5.13(11) | 0 | -1200 | [6] |

(*) - the value of coefficients for K₀ (low pressure limit) are presented

(**) - the rate constants is defined by presented equations

| Reaction | The rate constants, (cm ³ /mol) ^{m-1} ·s ⁻¹ | |
|----------|--|--|
| | Symbol | Equation |
| 87 (*) | | $\lg(K_{\downarrow}/K_0) = -2.54 + 4.6 \cdot 10^{-3}T - 2.96 \cdot 10^{-6}T^2 + 5.06 \cdot 10^{-10}T^3$ |
| 165 (*) | | $\lg(K_{\downarrow}/K_0) = -3 + 4.68 \cdot 10^{-3}T - 2.51 \cdot 10^{-6}T^2 + 4.5 \cdot 10^{-10}T^3$ $\lg(K_{\downarrow}/K_0) = -3 + 4.68 \cdot 10^{-3}T - 2.51 \cdot 10^{-6}T^2 + 4.5 \cdot 10^{-10}T^3$ |
| 206 (*) | | $\lg(K_{\downarrow}/K_0) = -0.54 + 8.68 \cdot 10^{-4}T - 3.34 \cdot 10^{-7}T^2$ $\lg(K_{\downarrow}/K_0) = -0.536 - 8.68 \cdot 10^{-4}T - 3.34 \cdot 10^{-7}T^2$ |
| 103 (**) | K _a | $K_a + K_b = 3.612 \cdot 10^{13}$ |
| 123 (**) | K _b | $\lg(K_b/K_a) = -1.915 + 2.69 \cdot 10^{-3}T - 2.35 \cdot 10^{-7}T^2$ |
| 178 (**) | | $K_{\downarrow} = 1.75 \cdot 10^{13} \cdot \exp(-1600/T) - 9.03 \cdot 10^{12} \cdot \exp(-2285/T)$ |
| 334 (**) | | $K_{\downarrow} = 2.53 \cdot 10^{13} \cdot 10^{f(T)} / (1 + 1 / (1.1 \cdot 10^{-28} \cdot T^{8.52} \exp(1248/T)))$ $f(T) = -0.177 + 6.69 \cdot 10^{-4}T - 6.04 \cdot 10^{-7}T^2 + 1.07 \cdot 10^{-10}T^3$ |
| 386 (**) | | $K_{\downarrow} = 1.5 \cdot 10^{13} / (1 + 2.5 \cdot 10^{-36} \cdot T^{11.25} \exp(3289/T))$ |
| 389 (**) | | $K_{\downarrow} = 9.632 \cdot 10^{12} / (1 + 1.3 \cdot 10^{-27} \cdot T^{8.07} \exp(1315/T))$ |

Table 2. The mixture composition for air+thermal destruction of the $n\text{-C}_8\text{H}_{18}$ with equivalence ratio $\alpha=1; 0.5; 0.25$ under $T_0=1000\text{ K}$, $P_0=1\text{ MPa}$

| | H ₂ | CH ₄ | C ₂ H ₄ | C ₂ H ₆ | C ₃ H ₆ | C ₃ H ₈ | C ₄ H ₆ | C ₄ H ₈ | C ₄ H ₁₀ | O ₂ | N ₂ |
|---------------|----------------|-----------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|--------------------------------|----------------|----------------|
| $\alpha=1$ | 5.716(-3) | 1.297(-2) | 1.7587(-2) | 5.335(-3) | 3.14(-3) | 2.998(-3) | 2.215(-3) | 8.79(-4) | 7.838(-3) | 0.197757 | 0.743565 |
| $\alpha=0.5$ | 2.944(-3) | 6.681(-3) | 9.059(-3) | 2.748(-3) | 1.618(-3) | 1.544(-3) | 1.141(-3) | 4.53(-4) | 4.038(-3) | 0.203734 | 0.76604 |
| $\alpha=0.25$ | 1.495(-3) | 3.392(-3) | 4.599(-3) | 1.395(-3) | 8.21(-4) | 7.84(-4) | 5.79(-4) | 2.3(-4) | 2.05(-3) | 0.20686 | 0.777795 |

$A(-n)$ corresponds $A \cdot 10^{-n}$

Table 3. The variation of the temperature and gas composition with time for the combustion of the destruction products of C₈H₁₈+air and CH₄+air with $\alpha=0.25$, P₀=1 MPa, T₀=1000 K.

| | detr. C ₈ H ₁₈ | CH ₄ | detr. C ₈ H ₁₈ | CH ₄ | detr. C ₈ H ₁₈ | CH ₄ | detr. C ₈ H ₁₈ | CH ₄ |
|-------------------------------|---|-----------------|---|-----------------|---|-----------------|---|-----------------|
| | τ_{in} | | $\tau(T_{max})$ | | | | τ_{in} | τ_{eq} |
| t,s | 8.12(-3) | 8.12(-3) | 9.36(-3) | 9.36(-3) | 6.63(-2) | 6.63(-2) | 20 | 30 |
| T,K | 1513.2 | 1000.1 | 1609.6 | 1000.2 | 1606.8 | 1489.34 | 1561.5 | 1536.6 |
| H ₂ O | 3.95(-2) | 1.98(-5) | 3.99(-2) | 2.52(-5) | 3.97(-2) | 5.06(-2) | 3.41(-2) | 4.61(-2) |
| O ₂ | 1.59(-1) | 2.05(-1) | 1.54(-1) | 2.05(-1) | 1.54(-1) | 1.58(-1) | 1.38(-1) | 1.40(-1) |
| H ₂ | 3.19(-5) | 1.14(-7) | 7.87(-7) | 1.48(-7) | 1.14(-5) | 4.68(-5) | 4.52(-4) | 4.10(-4) |
| OH | 3.43(-4) | 1.70(-9) | 1.47(-4) | 1.91(-9) | 4.40(-4) | 3.29(-4) | 4.37(-4) | 4.63(-4) |
| H | 9.35(-6) | 3.44(-11) | 8.27(-8) | 3.97(-11) | 2.75(-6) | 8.75(-6) | 9.06(-6) | 9.66(-6) |
| O | 1.43(-4) | 8.32(-10) | 1.01(-5) | 9.77(-10) | 8.99(-5) | 1.16(-4) | 4.32(-5) | 4.75(-5) |
| N ₂ | 7.69(-1) | 7.70(-1) | 7.74(-1) | 7.70(-1) | 7.74(-1) | 7.65(-1) | 7.69(-1) | 7.65(-1) |
| HO ₂ | 3.60(-6) | 2.50(-8) | 1.14(-6) | 3.04(-8) | 1.08(-6) | 3.64(-6) | 6.76(-7) | 7.73(-7) |
| H ₂ O ₂ | 2.13(-6) | 1.61(-8) | 1.61(-7) | 1.99(-8) | 1.36(-6) | 2.51(-6) | 2.06(-6) | 2.96(-6) |
| N | 2.22(-12) | 4.00(-23) | 3.19(-13) | 4.72(-23) | 4.23(-12) | 9.49(-13) | 1.69(-11) | 1.49(-11) |
| NO | 4.93(-8) | 1.56(-16) | 5.09(-7) | 2.32(-16) | 1.77(-4) | 3.07(-8) | 1.11(-2) | 9.49(-3) |
| NO ₂ | 1.02(-8) | 2.00(-17) | 9.88(-7) | 4.06(-17) | 1.01(-4) | 6.80(-9) | 3.68(-3) | 3.21(-3) |
| HNO ₂ | 3.81(-8) | 1.36(-19) | 4.57(-7) | 2.57(-19) | 1.79(-4) | 2.34(-8) | 1.11(-2) | 9.65(-3) |
| N ₂ O | 4.64(-6) | 3.28(-9) | 3.91(-5) | 3.95(-9) | 2.92(-5) | 4.44(-6) | 1.33(-5) | 1.08(-5) |
| NH | 1.92(-11) | 2.83(-21) | 2.38(-12) | 3.94(-21) | 5.11(-11) | 1.50(-11) | 4.34(-10) | 4.04(-10) |
| NH ₂ | 8.40(-13) | 2.03(-21) | 1.02(-13) | 2.65(-21) | 1.40(-12) | 8.73(-13) | 1.59(-11) | 1.70(-11) |
| NH ₃ | 1.15(-12) | 9.94(-23) | 3.99(-13) | 1.75(-22) | 1.85(-12) | 1.52(-12) | 1.80(-11) | 2.27(-11) |
| N ₂ H | 4.70(-9) | 1.27(-14) | 4.54(-11) | 1.47(-14) | 1.47(-9) | 4.30(-9) | 4.63(-9) | 4.79(-9) |
| N ₂ H ₂ | 3.74(-13) | 5.85(-21) | 3.48(-17) | 8.46(-21) | 2.15(-14) | 3.61(-13) | 2.80(-13) | 3.26(-13) |
| N ₂ H ₃ | 1.30(-16) | 8.85(-26) | 6.31(-22) | 1.50(-25) | 1.18(-18) | 1.42(-16) | 3.68(-17) | 5.70(-17) |
| N ₂ H ₄ | 9.14(-19) | 4.89(-28) | 3.17(-24) | 1.08(-27) | 5.46(-21) | 1.16(-18) | 3.01(-19) | 5.63(-19) |
| HNO | 4.02(-12) | 4.39(-23) | 1.19(-12) | 6.12(-23) | 2.22(-9) | 2.76(-12) | 2.01(-7) | 1.79(-7) |
| O ₃ | 1.77(-7) | 1.11(-9) | 7.80(-9) | 1.35(-9) | 6.59(-8) | 1.62(-7) | 3.56(-8) | 4.45(-8) |
| HNO ₃ | 3.22(-10) | 7.66(-22) | 6.96(-9) | 1.77(-21) | 2.15(-6) | 2.43(-10) | 1.04(-4) | 1.14(-4) |
| NO ₃ | 5.79(-12) | 1.92(-21) | 2.96(-11) | 3.54(-21) | 2.51(-8) | 3.99(-12) | 1.87(-6) | 1.95(-6) |
| HNO ₄ | 8.30(-29) | 0 | 1.08(-25) | 0 | 3.65(-24) | 5.88(-29) | 4.66(-23) | 3.30(-23) |
| C | 1.38(-9) | 2.30(-20) | 1.45(-12) | 3.72(-20) | 2.42(-22) | 1.08(-10) | 2.44(-25) | 1.82(-25) |
| CH ₄ | 4.76(-7) | 2.56(-2) | 3.57(-17) | 2.56(-2) | 6.13(-23) | 5.31(-6) | 2.49(-21) | 2.85(-21) |
| CH ₃ | 3.36(-7) | 6.38(-7) | 5.42(-17) | 6.95(-7) | 2.67(-22) | 2.07(-6) | 6.98(-21) | 7.21(-21) |
| C ₂ H ₆ | 6.88(-10) | 3.30(-6) | 3.80(-29) | 4.44(-6) | 0 | 3.26(-8) | 0 | 0 |
| C ₂ H ₅ | 2.95(-12) | 2.32(-12) | 2.25(-28) | 3.33(-12) | 0 | 7.20(-11) | 0 | 0 |
| C ₂ H ₄ | 1.47(-7) | 1.79(-8) | 3.27(-21) | 2.84(-8) | 6.75(-29) | 6.52(-7) | 2.10(-27) | 4.12(-28) |
| C ₂ H ₃ | 3.47(-9) | 3.43(-15) | 6.37(-22) | 5.97(-15) | 1.58(-29) | 1.04(-8) | 3.55(-28) | 3.46(-29) |
| C ₂ H ₂ | 9.75(-6) | 1.90(-11) | 8.25(-16) | 3.81(-11) | 7.33(-25) | 4.37(-5) | 3.64(-24) | 2.70(-25) |
| HCO | 1.30(-8) | 3.21(-12) | 1.19(-14) | 4.21(-12) | 1.85(-12) | 4.71(-8) | 1.89(-11) | 1.49(-11) |
| CH ₂ | 1.58(-8) | 1.19(-12) | 2.30(-15) | 1.54(-12) | 1.65(-24) | 6.63(-8) | 1.72(-25) | 2.28(-25) |
| CO ₂ | 1.93(-2) | 1.11(-10) | 3.15(-2) | 2.02(-10) | 3.15(-2) | 1.45(-2) | 3.17(-2) | 2.58(-2) |
| HCN | 2.32(-9) | 5.91(-21) | 4.36(-13) | 9.50(-21) | 7.66(-16) | 2.03(-10) | 1.06(-15) | 6.41(-16) |
| C ₂ N ₂ | 2.62(-17) | 0 | 3.59(-19) | 0 | 2.48(-28) | 1.04(-19) | 1.95(-29) | 7.76(-30) |
| CO | 1.19(-2) | 6.71(-7) | 3.44(-6) | 1.01(-6) | 1.75(-5) | 1.08(-2) | 5.09(-5) | 3.69(-5) |

| | | | | | | | | |
|---|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| NCO | 4.12(-11) | 2.73(-22) | 5.46(-14) | 5.58(-22) | 9.86(-15) | 3.55(-12) | 2.63(-15) | 1.75(-15) |
| CH ₃ O | 2.29(-10) | 9.99(-11) | 3.25(-20) | 1.14(-10) | 9.73(-22) | 1.40(-9) | 3.36(-20) | 3.33(-20) |
| CH ₂ O | 5.50(-7) | 1.50(-5) | 2.42(-16) | 1.85(-5) | 1.09(-14) | 2.90(-6) | 9.39(-14) | 7.82(-14) |
| CH ₃ OH | 2.79(-9) | 3.18(-9) | 2.62(-19) | 4.15(-9) | 8.78(-24) | 1.96(-8) | 3.11(-22) | 3.03(-22) |
| CH | 8.29(-11) | 6.58(-23) | 2.40(-19) | 7.18(-23) | 5.73(-23) | 1.64(-11) | 1.64(-25) | 1.02(-25) |
| CH ₂ OH | 1.82(-10) | 4.10(-15) | 5.37(-21) | 6.01(-15) | 9.29(-22) | 1.31(-9) | 2.98(-20) | 2.86(-20) |
| CN | 2.34(-13) | 8.31(-29) | 1.16(-16) | 1.35(-28) | 2.51(-18) | 1.79(-14) | 4.33(-19) | 2.93(-19) |
| C ₂ | 1.07(-14) | 0 | 7.74(-28) | 0 | 0 | 1.34(-15) | 0 | 0 |
| CH ₃ O ₂ | 7.52(-11) | 1.52(-8) | 8.00(-21) | 1.65(-8) | 3.76(-26) | 5.22(-10) | 1.08(-24) | 1.26(-24) |
| CH ₂ CO | 9.30(-8) | 2.52(-14) | 7.57(-18) | 4.78(-14) | 1.23(-25) | 4.37(-7) | 9.07(-24) | 5.11(-24) |
| CH ₃ CO | 5.57(-12) | 4.31(-16) | 2.10(-25) | 7.01(-16) | 0.0 | 1.15(-11) | 6.79(-29) | 5.27(-29) |
| CH ₃ CHO | 2.35(-9) | 1.96(-12) | 1.83(-22) | 3.16(-12) | 4.70(-30) | 3.21(-9) | 1.23(-28) | 2.37(-29) |
| CH ₃ O ₂ CH ₃ | 8.52(-22) | 2.07(-16) | 0 | 2.45(-16) | 0 | 3.90(-20) | 0 | 0 |
| C ₂ H | 1.84(-8) | 2.22(-21) | 2.11(-19) | 4.88(-21) | 4.74(-27) | 4.45(-9) | 3.12(-25) | 2.86(-28) |
| C ₂ HO | 2.73(-9) | 1.97(-15) | 5.61(-20) | 5.19(-15) | 5.94(-28) | 1.89(-6) | 3.53(-26) | 4.01(-24) |
| CH ₃ O ₂ H | 2.91(-15) | 3.20(-12) | 1.05(-25) | 3.53(-12) | 5.65(-27) | 2.24(-14) | 2.84(-25) | 3.71(-25) |
| C ₂ N | 7.94(-14) | 0 | 8.20(-14) | 0 | 8.17(-14) | 1.99(-16) | 0 | 0 |
| C ₃ H ₅ | 5.00(-9) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₆ | 6.66(-11) | - | 0 | - | 0 | - | 0 | - |
| C ₄ H ₆ | 1.30(-7) | - | 0 | - | 0 | - | 0 | - |
| C ₄ H ₈ | 5.25(-10) | - | 0 | - | 0 | - | 0 | - |
| C ₄ H ₁₀ | 6.85(-17) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₈ | 6.20(-15) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₄ | 3.23(-7) | - | 0 | - | 0 | - | 0 | - |
| nC ₃ H ₇ | 9.18(-15) | - | 0 | - | 0 | - | 0 | - |
| iC ₃ H ₇ | 1.68(-15) | - | 0 | - | 0 | - | 0 | - |
| nC ₄ H ₉ | 9.81(-20) | - | 0 | - | 0 | - | 0 | - |
| sC ₄ H ₉ | 4.55(-19) | - | 0 | - | 0 | - | 0 | - |
| CH ₃ CO ₃ | 3.53(-14) | - | 6.11(-28) | - | 0 | - | 0 | - |
| CH ₃ CO ₃ H | 8.62(-13) | - | 1.13(-30) | - | 0 | - | 0 | - |
| C ₂ H ₅ O | 6.92(-20) | - | 0 | - | 0 | - | 0 | - |
| C ₂ H ₅ O ₂ | 4.56(-15) | - | 0 | - | 0 | - | 0 | - |
| C ₂ H ₅ O ₂ H | 5.82(-22) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₅ O | 2.60(-16) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₅ O ₂ | 2.18(-12) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₅ O ₂ H | 4.55(-20) | - | 0 | - | 0 | - | 0 | - |
| C ₃ H ₆ O | 1.23(-15) | - | 0 | - | 0 | - | 0 | - |
| nC ₃ H ₇ O | 2.14(-22) | - | 0 | - | 0 | - | 0 | - |
| nC ₃ H ₇ O ₂ | 1.42(-17) | - | 0 | - | 0 | - | 0 | - |
| nC ₃ H ₇ O ₂ H | 4.14(-25) | - | 0 | - | 0 | - | 0 | - |
| iC ₃ H ₇ O | 6.45(-23) | - | 0 | - | 0 | - | 0 | - |
| iC ₃ H ₇ O ₂ | 2.59(-18) | - | 0 | - | 0 | - | 0 | - |
| iC ₃ H ₇ O ₂ H | 5.30(-26) | - | 0 | - | 0 | - | 0 | - |

A(-n) corresponds A·10⁻ⁿ

Table 4. Gas composition and temperature in the different section of gas-turbine engine versus time under equilibrium gas composition at the exit plane of combustion chamber.

| | Combustion chamber | HPT | HPT-MPT Duct | MPT | LPT 1 | LPT 2 | LPT 3 | Exhaust Nozzle |
|--------------------------------|--------------------|-----------|--------------|-----------|-----------|-----------|-----------|----------------|
| t,ms | 0 | 0.43 | 1.25 | 1.8 | 2.31 | 2.64 | 3.1 | 4.3 |
| T,K | 1541 | 1337 | 1347 | 1125 | 921 | 743 | 674 | 598 |
| H ₂ O | 3.47(-2) | 3.63(-2) | 3.65(-2) | 3.67(-2) | 3.68(-2) | 3.68(-2) | 3.68(-2) | 3.68(-2) |
| O ₂ | 1.39(-1) | 1.39(-1) | 1.39(-1) | 1.39(-1) | 1.39(-1) | 1.39(-1) | 1.39(-1) | 1.39(-1) |
| H ₂ | 4.08(-4) | 2.07(-4) | 1.91(-4) | 1.80(-4) | 1.77(-4) | 1.77(-4) | 1.77(-4) | 1.77(-4) |
| OH | 3.64(-4) | 1.10(-4) | 9.23(-5) | 7.67(-6) | 2.44(-7) | 7.13(-9) | 5.88(-10) | 7.24(-11) |
| H | 5.05(-6) | 1.38(-6) | 1.17(-6) | 7.89(-8) | 2.14(-9) | 5.25(-11) | 4.67(-12) | 2.66(-13) |
| O | 3.14(-5) | 3.02(-6) | 2.50(-6) | 4.64(-8) | 2.75(-10) | 1.11(-12) | 1.89(-14) | 6.29(-16) |
| N ₂ | 7.69(-1) | 7.68(-1) | 7.68(-1) | 7.67(-1) | 7.67(-1) | 7.67(-1) | 7.67(-1) | 7.67(-1) |
| HO ₂ | 3.05(-7) | 7.62(-8) | 6.46(-8) | 3.33(-9) | 6.25(-11) | 1.17(-12) | 9.07(-14) | 6.36(-15) |
| H ₂ O ₂ | 1.43(-6) | 8.71(-7) | 5.55(-7) | 1.24(-7) | 3.69(-8) | 3.62(-8) | 3.62(-8) | 3.62(-8) |
| N | 7.18(-12) | 1.97(-13) | 1.69(-13) | 4.25(-15) | 3.16(-16) | 1.09(-17) | 1.10(-18) | 7.49(-20) |
| NO | 1.05(-2) | 1.26(-2) | 1.28(-2) | 1.30(-2) | 1.30(-2) | 1.30(-2) | 1.30(-2) | 1.30(-2) |
| NO ₂ | 3.58(-3) | 4.29(-3) | 4.24(-3) | 4.56(-3) | 4.65(-3) | 4.66(-3) | 4.66(-3) | 4.66(-3) |
| HNO ₂ | 1.02(-2) | 7.37(-3) | 7.16(-3) | 6.75(-3) | 6.62(-3) | 6.61(-3) | 6.61(-3) | 6.61(-3) |
| N ₂ O | 1.38(-5) | 1.36(-5) | 1.28(-5) | 1.25(-5) | 1.25(-5) | 1.25(-5) | 1.25(-5) | 1.25(-5) |
| NH | 1.73(-10) | 5.45(-12) | 4.38(-12) | 4.08(-14) | 1.23(-16) | 1.71(-19) | 6.19(-22) | 1.99(-23) |
| NH ₂ | 9.18(-12) | 1.56(-13) | 9.61(-14) | 3.76(-16) | 1.76(-18) | 1.40(-20) | 4.11(-22) | 2.99(-23) |
| NH ₃ | 1.71(-11) | 6.42(-13) | 2.93(-13) | 1.82(-13) | 1.70(-13) | 1.70(-13) | 1.70(-13) | 1.70(-13) |
| N ₂ H | 1.16(-9) | 2.95(-10) | 2.58(-10) | 9.77(-12) | 1.68(-13) | 4.19(-15) | 1.90(-16) | 4.72(-17) |
| N ₂ H ₂ | 2.29(-13) | 1.12(-14) | 7.60(-15) | 3.48(-15) | 2.86(-15) | 2.84(-15) | 2.84(-15) | 2.84(-15) |
| N ₂ H ₃ | 1.79(-17) | 9.62(-19) | 5.39(-19) | 9.40(-20) | 1.94(-20) | 1.08(-20) | 9.16(-21) | 8.55(-21) |
| N ₂ H ₄ | 1.72(-19) | 5.33(-21) | 2.33(-21) | 5.61(-22) | 2.09(-22) | 2.08(-22) | 2.08(-22) | 2.08(-22) |
| HNO | 6.74(-8) | 1.34(-8) | 1.19(-8) | 4.27(-10) | 5.86(-12) | 6.85(-14) | 3.74(-15) | 1.38(-16) |
| O ₃ | 1.83(-8) | 4.53(-9) | 3.58(-9) | 2.25(-10) | 7.71(-12) | 2.38(-13) | 8.18(-15) | 3.03(-15) |
| HNO ₃ | 6.85(-5) | 8.11(-5) | 6.30(-5) | 3.03(-5) | 1.23(-5) | 1.09(-5) | 1.09(-5) | 1.09(-5) |
| NO ₃ | 1.43(-6) | 2.56(-6) | 1.52(-6) | 6.40(-7) | 1.81(-7) | 1.20(-7) | 9.03(-8) | 8.27(-8) |
| HNO ₄ | 4.54(-23) | 1.04(-23) | 1.53(-24) | 1.08(-24) | 1.03(-24) | 1.03(-24) | 1.03(-24) | 1.03(-24) |
| C | 3.14(-25) | 1.03(-25) | 2.73(-26) | 1.24(-26) | 1.01(-26) | 8.83(-27) | 7.82(-27) | 6.98(-27) |
| CH ₄ | 2.40(-21) | 3.65(-23) | 7.52(-24) | 5.27(-24) | 5.23(-24) | 5.25(-24) | 5.25(-24) | 5.25(-24) |
| CH ₃ | 5.66(-21) | 3.95(-23) | 1.14(-23) | 1.59(-24) | 6.10(-25) | 3.01(-25) | 5.53(-26) | 1.04(-26) |
| HCO | 4.87(-12) | 9.79(-13) | 4.87(-13) | 1.78(-14) | 2.42(-16) | 2.34(-18) | 1.14(-19) | 3.59(-21) |
| CH ₂ | 1.87(-25) | 1.46(-25) | 8.90(-26) | 6.51(-26) | 6.63(-26) | 6.76(-26) | 6.86(-26) | 6.94(-26) |
| CO ₂ | 3.17(-2) | 3.17(-2) | 3.17(-2) | 3.17(-2) | 3.17(-2) | 3.17(-2) | 3.17(-2) | 3.17(-2) |
| CO | 5.06(-5) | 3.02(-5) | 1.74(-5) | 1.43(-5) | 1.42(-5) | 1.42(-5) | 1.42(-5) | 1.42(-5) |
| CH ₃ O | 6.49(-21) | 2.78(-22) | 1.19(-22) | 2.89(-24) | 1.96(-25) | 2.93(-26) | 1.78(-27) | 6.88(-28) |
| CH ₂ O | 6.01(-14) | 3.31(-15) | 1.73(-15) | 2.36(-16) | 1.36(-16) | 1.34(-16) | 1.34(-16) | 1.34(-16) |
| CH ₃ OH | 2.53(-22) | 2.29(-24) | 8.84(-25) | 2.96(-25) | 2.44(-25) | 2.45(-25) | 2.45(-25) | 2.45(-25) |
| CH | 7.56(-26) | 2.10(-29) | 1.04(-29) | 0 | 0 | 0 | 0 | 0 |
| CH ₂ OH | 8.76(-21) | 1.58(-22) | 6.82(-23) | 7.27(-25) | 1.21(-26) | 3.68(-28) | 1.16(-29) | 4.12(-30) |
| CH ₃ O ₂ | 1.06(-24) | 2.26(-26) | 6.12(-27) | 4.76(-27) | 2.18(-26) | 2.37(-25) | 4.78(-25) | 5.23(-25) |

A(-n) corresponds A · 10⁻ⁿ

Table 5. Gas composition and temperature in the different section of gas-turbine engine versus time under nonequilibrium gas composition at the exit plane of combustion chamber.

| | Combustion chamber | HPT | HPT-MPT Duct | MPT | LPT 1 | LPT 2 | LPT 3 | Exhaust Nozzle |
|--------------------------------|--------------------|-----------|--------------|-----------|-----------|-----------|-----------|----------------|
| t, ms | 0 | 0.43 | 1.25 | 1.8 | 2.31 | 2.64 | 3.1 | 4.3 |
| T, K | 1541 | 1336 | 1346 | 1100 | 901 | 736 | 614 | 590 |
| H ₂ O | 3.97(-2) | 3.99(-2) | 3.99(-2) | 3.99(-2) | 3.99(-2) | 4.00(-2) | 4.00(-2) | 4.00(-2) |
| O ₂ | 1.54(-1) | 1.54(-1) | 1.54(-1) | 1.54(-1) | 1.54(-1) | 1.54(-1) | 1.54(-1) | 1.54(-1) |
| H ₂ | 6.79(-6) | 2.77(-6) | 2.28(-6) | 1.90(-6) | 1.54(-6) | 1.48(-6) | 1.48(-6) | 1.47(-6) |
| OH | 3.68(-4) | 1.14(-4) | 1.05(-4) | 4.26(-5) | 1.27(-5) | 2.54(-6) | 9.00(-7) | 2.98(-7) |
| H | 1.58(-6) | 3.95(-7) | 3.27(-7) | 1.63(-7) | 2.44(-8) | 1.16(-9) | 1.94(-10) | 3.41(-11) |
| O | 6.36(-5) | 1.71(-5) | 1.43(-5) | 6.87(-6) | 1.87(-6) | 3.12(-7) | 1.12(-7) | 1.83(-8) |
| N ₂ | 7.74(-1) | 7.74(-1) | 7.74(-1) | 7.74(-1) | 7.74(-1) | 7.74(-1) | 7.74(-1) | 7.74(-1) |
| HO ₂ | 8.61(-7) | 2.14(-7) | 1.99(-7) | 1.27(-7) | 4.10(-8) | 6.05(-9) | 2.26(-9) | 7.26(-10) |
| H ₂ O ₂ | 9.80(-7) | 9.04(-7) | 7.13(-7) | 1.56(-6) | 1.20(-6) | 1.10(-6) | 1.09(-6) | 1.08(-6) |
| N | 2.23(-12) | 4.98(-14) | 4.18(-14) | 2.19(-15) | 4.58(-17) | 6.61(-19) | 7.48(-20) | 6.51(-21) |
| NO | 7.12(-5) | 9.10(-5) | 9.13(-5) | 1.01(-4) | 1.03(-4) | 1.04(-4) | 1.04(-4) | 1.04(-4) |
| NO ₂ | 5.13(-5) | 4.92(-5) | 5.19(-5) | 4.61(-5) | 4.55(-5) | 4.49(-5) | 4.49(-5) | 4.49(-5) |
| HNO ₂ | 7.20(-5) | 5.51(-5) | 5.23(-5) | 4.72(-5) | 4.33(-5) | 4.19(-5) | 4.17(-5) | 4.16(-5) |
| N ₂ O | 3.35(-5) | 3.07(-5) | 2.88(-5) | 2.79(-5) | 2.79(-5) | 2.78(-5) | 2.78(-5) | 2.78(-5) |
| NH | 3.17(-11) | 3.01(-12) | 2.47(-12) | 3.38(-13) | 1.68(-14) | 5.57(-16) | 1.52(-16) | 1.26(-17) |
| NH ₂ | 9.30(-13) | 1.17(-13) | 9.18(-14) | 4.69(-14) | 6.50(-15) | 1.76(-15) | 7.17(-16) | 1.22(-16) |
| NH ₃ | 1.47(-12) | 3.42(-13) | 2.59(-13) | 2.14(-13) | 1.89(-13) | 1.85(-13) | 1.84(-13) | 1.84(-13) |
| N ₂ H | 7.26(-10) | 8.37(-11) | 7.16(-11) | 1.72(-11) | 1.85(-12) | 4.33(-14) | 8.26(-15) | 2.24(-15) |
| N ₂ H ₂ | 7.54(-15) | 7.23(-16) | 5.01(-16) | 3.17(-16) | 1.50(-16) | 1.27(-16) | 1.25(-16) | 1.24(-16) |
| N ₂ H ₃ | 2.80(-19) | 1.07(-19) | 6.31(-20) | 3.00(-19) | 1.79(-19) | 1.49(-19) | 1.46(-19) | 1.45(-19) |
| N ₂ H ₄ | 1.14(-21) | 4.69(-22) | 2.57(-22) | 2.05(-21) | 9.33(-22) | 8.15(-22) | 7.69(-22) | 7.32(-22) |
| HNO | 5.64(-10) | 6.12(-11) | 5.23(-11) | 1.25(-11) | 1.52(-12) | 1.16(-13) | 2.64(-14) | 7.53(-15) |
| O ₃ | 4.67(-8) | 2.74(-8) | 2.19(-8) | 4.11(-8) | 6.05(-8) | 6.17(-8) | 7.41(-8) | 7.73(-8) |
| HNO ₃ | 9.20(-7) | 9.65(-7) | 8.82(-7) | 1.98(-6) | 1.72(-6) | 1.04(-6) | 3.70(-7) | 2.23(-7) |
| NO ₃ | 1.74(-8) | 2.90(-8) | 2.21(-8) | 3.14(-7) | 2.43(-6) | 4.88(-6) | 5.75(-6) | 5.98(-6) |
| HNO ₄ | 2.27(-24) | 1.43(-25) | 1.95(-26) | 1.09(-26) | 8.23(-27) | 7.78(-27) | 7.72(-27) | 7.68(-27) |
| C | 3.30(-22) | 3.15(-22) | 3.09(-22) | 3.07(-22) | 3.06(-22) | 3.06(-22) | 3.06(-22) | 3.05(-22) |
| CH ₄ | 1.48(-23) | 1.07(-24) | 2.90(-25) | 2.94(-25) | 2.77(-25) | 2.74(-25) | 2.73(-25) | 2.73(-25) |
| CH ₃ | 5.71(-23) | 1.99(-24) | 7.14(-25) | 6.60(-25) | 2.03(-25) | 4.40(-26) | 2.32(-27) | 5.67(-28) |
| HCO | 5.61(-13) | 6.08(-14) | 2.86(-14) | 6.89(-15) | 4.36(-16) | 8.21(-18) | 5.64(-19) | 8.13(-20) |
| CH ₂ | 2.01(-24) | 5.48(-24) | 6.98(-24) | 7.54(-24) | 7.73(-24) | 7.98(-24) | 8.17(-24) | 8.62(-24) |
| CO ₂ | 3.15(-2) | 3.15(-2) | 3.15(-2) | 3.15(-2) | 3.15(-2) | 3.15(-2) | 3.15(-2) | 3.15(-2) |
| CO | 1.19(-5) | 6.93(-6) | 3.87(-6) | 3.14(-6) | 3.01(-6) | 2.99(-6) | 2.99(-6) | 2.99(-6) |
| CH ₃ O | 2.24(-22) | 6.19(-24) | 2.41(-24) | 1.23(-24) | 2.02(-25) | 1.84(-26) | 3.79(-27) | 4.67(-28) |
| CH ₂ O | 4.48(-15) | 2.59(-16) | 1.26(-16) | 4.08(-17) | 1.07(-17) | 5.43(-18) | 5.05(-18) | 4.87(-18) |
| CH ₃ OH | 2.36(-24) | 4.64(-26) | 1.75(-26) | 3.04(-26) | 4.30(-26) | 9.59(-26) | 1.23(-25) | 1.38(-25) |
| CH | 2.61(-25) | 5.21(-29) | 4.26(-29) | 7.36(-30) | 1.51(-30) | 0 | 0 | 0 |
| CH ₂ OH | 2.17(-22) | 3.45(-24) | 1.39(-24) | 2.38(-25) | 9.59(-27) | 5.78(-28) | 3.42(-28) | 1.71(-28) |
| CH ₃ O ₂ | 9.39(-27) | 1.27(-27) | 4.24(-28) | 3.06(-27) | 1.55(-26) | 7.74(-26) | 9.24(-26) | 8.20(-26) |

A(-n) corresponds A·10⁻ⁿ

Table 6. The chemical reactions list for plume chemistry model.

| № | Reactions | Rate constants | | |
|---|--|---|----------|----------|
| | | $K = AT^n \exp\left(\frac{E}{T}\right) (\text{cm}^3)^{m-1} \text{s}^{-1}$ | | |
| | | <i>A</i> | <i>n</i> | <i>E</i> |
| 1 | 2 | 3 | 4 | 5 |
| Reactions with H, H ₂ , H ₂ O, HO ₂ , H ₂ O ₂ , OH, O, O ₂ , O ₃ | | | | |
| 1. | 2H+M=H ₂ +M | 9.11(-33) | -1.3 | 0 |
| 2. | 2O+M=O ₂ +M | 3.80(-30) | -1.0 | -170 |
| 3. | H+O+M=OH+M | 1.96(-29) | -1.0 | 0 |
| 4. | OH+H+M=H ₂ O+M | 6.07(-26) | -2.0 | 0 |
| 5. | O+H ₂ =OH+H | 9(-18) | 0 | 0 |
| 6. | O+OH=O ₂ +H | 2.3(-11) | 0 | 110 |
| 7. | OH+H=H ₂ +O | 1.38(-14) | 1 | -3500 |
| 8. | OH+H ₂ =H ₂ O+H | 7.7(-12) | 0 | -2100 |
| 9. | 2OH=H ₂ O+O | 4.2(-12) | 0 | -240 |
| 10. | H+O ₂ +M=HO ₂ +M, M=O ₂ | 1.77(-29) | -1 | 0 |
| 11. | H+O ₂ +M=HO ₂ +M, M=N ₂ | 1.77(-29) | -1 | 0 |
| 12. | H+HO ₂ =H ₂ +O ₂ | 5.6(-12) | 0 | 0 |
| 13. | H+HO ₂ =2OH | 7.2(-11) | 0 | 0 |
| 14. | H+HO ₂ =H ₂ O+O | 2.4(-12) | 0 | 0 |
| 15. | O+HO ₂ =OH+O ₂ | 2.9(-11) | 0 | 200 |
| 16. | OH+HO ₂ =H ₂ O+O ₂ | 4.8(-11) | 0 | 240 |
| 17. | 2OH+M=H ₂ O ₂ +M | 6.62(-29) | -0.8 | 0 |
| 18. | 2HO ₂ =H ₂ O ₂ +O ₂ | 2.20(-13) | 0 | 600 |
| 19. | H+H ₂ O ₂ =HO ₂ +H ₂ | 2.82(-12) | 0 | -1900 |
| 20. | H+H ₂ O ₂ =H ₂ O+OH | 8.31(-10) | 0 | -5000 |
| 21. | O+H ₂ O ₂ =H ₂ O+O ₂ | 1.40(-12) | 0 | -2130 |
| 22. | O+H ₂ O ₂ =OH+HO ₂ | 1.4(-12) | 0 | -2000 |
| 23. | OH+H ₂ O ₂ =H ₂ O+HO ₂ | 2.9(-12) | 0 | -160 |
| 24. | O+O ₂ +M=O ₃ +M, M=O ₂ | 5.58(-29) | -2 | 0 |
| 25. | O+O ₂ +M=O ₃ +M, M=N ₂ | 5.13(-29) | -2 | 0 |
| 26. | HO ₂ +O ₂ =O ₃ +OH | 1.50(-15) | 0 | 0 |
| 27. | O+O ₃ =2O ₂ | 8(-12) | 0 | -2060 |
| 28. | H+O ₃ =OH+O ₂ | 1.4(-10) | 0 | -480 |
| 29. | OH+O ₃ =HO ₂ +O ₂ | 1.9(-12) | 0 | -1000 |
| 30. | HO ₂ +O ₃ =OH+2O ₂ | 1.4(-14) | 0 | -600 |
| Reactions with N, NO, NO ₂ , NO ₃ , HNO, HNO ₂ , HNO ₃ , HNO ₄ , N ₂ O ₅ | | | | |
| 31. | N+O+M=NO+M | 2.76(-28) | -1.5 | 0 |
| 32. | 2N+M=N ₂ +M | 8.33(-34) | 0 | 500 |
| 33. | N+OH=NO+H | 3.8(-11) | 0 | 85 |
| 34. | N+O ₂ =NO+O | 4.4(-12) | 0 | -3220 |
| 35. | N+HO ₂ =NO+OH | 1.66(-11) | 0 | -1000 |
| 36. | N+O ₃ =NO+O ₂ | 1(-16) | 0 | 0 |
| 37. | N+NO=N ₂ +O | 3.1(-11) | 0 | 0 |
| 38. | O+NO+M=NO ₂ +M, M=O ₂ | 2.47(-27) | -1.8 | 0 |
| 39. | O+NO+M=NO ₂ +M, M=N ₂ | 9.19(-31) | -1.6 | 0 |
| 40. | NO+O ₃ =NO ₂ +O ₂ | 1.8(-12) | 0 | -1370 |
| 41. | HO ₂ +NO=OH+NO ₂ | 3.7(-12) | 0 | 240 |
| 42. | 2NO+O ₂ =2NO ₂ | 3.3(-39) | 0 | 530 |
| 43. | O+NO ₂ =NO+O ₂ | 5.5(-12) | 0 | 120 |

| 1 | 2 | 3 | 4 | 5 |
|---|--|----------------------------|------|--------|
| 44. | $\text{H}+\text{NO}_2=\text{OH}+\text{NO}$ | 5.8(-10) | 0 | -750 |
| 45. | $\text{N}+\text{NO}_2=2\text{NO}$ | 5.98(-12) | 0 | 0 |
| 46. | $\text{OH}+\text{NO}+\text{M}=\text{HNO}_2+\text{M}$, $\text{M}=\text{O}_2$ | 6.52(-25) | -2.4 | 0 |
| 47. | $\text{OH}+\text{NO}+\text{M}=\text{HNO}_2+\text{M}$, $\text{M}=\text{N}_2$ | 6.52(-25) | -2.4 | 0 |
| 48. | $\text{H}+\text{HNO}_2=\text{H}_2+\text{NO}_2$ | 8.31(-13) | 0.5 | -1500 |
| 49. | $\text{O}+\text{HNO}_2=\text{OH}+\text{NO}_2$ | 1.(-12) | 0 | -2000 |
| 50. | $\text{OH}+\text{HNO}_2=\text{H}_2\text{O}+\text{NO}_2$ | 1.8(-11) | 0 | -390 |
| 51. | $\text{H}+\text{NO}+\text{M}=\text{HNO}+\text{M}$ | 1.49(-32) | 0 | 300 |
| 52. | $\text{NO}+\text{HO}_2=\text{HNO}+\text{O}_2$ | 3.32(-13) | 0 | -1000 |
| 53. | $\text{HNO}+\text{H}=\text{NO}+\text{H}_2$ | 2.09(-11) | 0 | -2000 |
| 54. | $\text{HNO}+\text{O}=\text{NO}+\text{OH}$ | 1.44(-11) | 0.5 | -1000 |
| 55. | $\text{HNO}+\text{OH}=\text{NO}+\text{H}_2\text{O}$ | 2.09(-12) | 0.5 | -1000 |
| 56. | $\text{HNO}+\text{HO}_2=\text{NO}+\text{H}_2\text{O}_2$ | 5.25(-13) | 0.5 | -1000 |
| 57. | $\text{OH}+\text{NO}_2+\text{M}=\text{HNO}_3+\text{M}$ | 6.63(-32) | 0 | 1016 |
| 58. | $\text{HO}_2+\text{NO}_2+\text{M}=\text{HNO}_4+\text{M}$, $\text{M}=\text{O}_2$ | 1.27(-23) | -3.2 | 0 |
| 59. | $\text{HO}_2+\text{NO}_2+\text{M}=\text{HNO}_4+\text{M}$, $\text{M}=\text{N}_2$ | 1.52(-23) | -3.2 | 0 |
| 60. | $\text{HNO}_4+\text{M}=\text{HO}_2+\text{NO}_2+\text{M}$, $\text{M}=\text{O}_2$ | 3.6(-6) (s-1) | 0 | -10000 |
| 61. | $\text{HNO}_4+\text{M}=\text{HO}_2+\text{NO}_2+\text{M}$, $\text{M}=\text{N}_2$ | 5(-6) (s-1) | 0 | -10000 |
| 62. | $\text{OH}+\text{HNO}_4=\text{H}_2\text{O}+\text{NO}_2+\text{O}_2$ | 1.3(-12) | 0 | 380 |
| 63. | $\text{N}+\text{NO}_2=\text{N}_2\text{O}+\text{O}$ | 3(-12) | 0 | 0 |
| 64. | $\text{O}+\text{NO}_3=\text{O}_2+\text{NO}_2$ | 1(-11) | 0 | 0 |
| 65. | $\text{O}+\text{NO}_2+\text{M}=\text{NO}_3+\text{M}$, $\text{M}=\text{O}_2$ | 8.1(-27) | -2 | 0 |
| 66. | $\text{O}+\text{NO}_2+\text{M}=\text{NO}_3+\text{M}$, $\text{M}=\text{N}_2$ | 8.1(-27) | -2 | 0 |
| 67. | $\text{NO}+\text{NO}_3=2\text{NO}_2$ | 1.6(-11) | 0 | 150 |
| 68. | $\text{NO}_2+\text{O}_3=\text{NO}_3+\text{O}_2$ | 1.2(-13) | 0 | -1370 |
| 69. | $\text{OH}+\text{NO}_3=\text{HO}_2+\text{NO}_2$ | 2.3(-11) | 0 | 0 |
| 70. | $\text{OH}+\text{HNO}_3=\text{H}_2\text{O}+\text{NO}_3$ | 9.4(-15) | 0 | 778 |
| 71. | $\text{HO}_2+\text{NO}_3=\text{O}_2+\text{HNO}_3$ | 9.24(-13) | 0 | 0 |
| 72. | $\text{HO}_2+\text{NO}_3=\text{OH}+\text{NO}_2+\text{O}_2$ | 3.6(-12) | 0 | 0 |
| 73. | $\text{N}_2\text{O}+\text{OH}=\text{N}_2+\text{HO}_2$ | 1.04(-12) | 0 | -5000 |
| 74. | $\text{N}_2\text{O}+\text{H}=\text{N}_2+\text{OH}$ | 1.26(-10) | 0 | -7600 |
| 75. | $\text{HNO}_3+\text{O}=\text{OH}+\text{NO}_3$ | 1.00(-12) | 0 | -4000 |
| 76. | $\text{NO}_3+\text{H}=\text{NO}_2+\text{OH}$ | 5.81(-10) | 0 | -750 |
| 77. | $\text{NO}_2+\text{NO}_3+\text{M}=\text{N}_2\text{O}_5+\text{M}$, $\text{M}=\text{O}_2$ | 5.3(-20) | -4.1 | 0 |
| 78. | $\text{NO}_2+\text{NO}_3+\text{M}=\text{N}_2\text{O}_5+\text{M}$, $\text{M}=\text{N}_2$ | 5.3(-20) | -4.1 | 0 |
| 79. | $\text{N}_2\text{O}_5+\text{M}=\text{NO}_2+\text{NO}_3+\text{M}$, $\text{M}=\text{O}_2$ | 1.74(8) (s ⁻¹) | -4.4 | -11080 |
| 80. | $\text{N}_2\text{O}_5+\text{M}=\text{NO}_2+\text{NO}_3+\text{M}$, $\text{M}=\text{N}_2$ | 1.74(8) (s ⁻¹) | -4.4 | -11080 |
| 81. | $\text{N}_2\text{O}_5+\text{H}_2\text{O}=2\text{HNO}_3$ | 2(-21) | 0 | 0 |
| Reactions with CH_3 , CH_4 , HCO , CO , CH_2O , CH_3O , CH_3OH , CH_3O_2 , $\text{CH}_3\text{O}_2\text{H}$, CH_3 | | | | |
| 82. | $\text{CH}_3+\text{O}=\text{CH}_2\text{O}+\text{H}$ | 1.1(-10) | 0 | 0 |
| 83. | $\text{CH}_3+\text{H}+\text{M}=\text{CH}_4+\text{M}$ | 7.78(-37) | 1 | 9828 |
| 84. | $\text{CH}_3+\text{OH}=\text{CH}_2\text{O}+\text{H}_2$ | 1.32(-11) | 0 | 0 |
| 85. | $\text{CH}_3+\text{OH}=\text{CH}_4+\text{O}$ | 5.90(-20) | 2.2 | -1976 |
| 86. | $\text{CH}_3+\text{HO}_2=\text{CH}_4+\text{O}_2$ | 1.66(-12) | 0 | -202 |
| 87. | $\text{CH}_3+\text{O}_2=\text{CH}_2\text{O}+\text{OH}$ | 5(-17) | 0 | 0 |
| 88. | $\text{CH}_3+\text{O}_2=\text{CH}_3\text{O}+\text{O}$ | 5.4(-12) | 0 | -220 |
| 89. | $\text{CH}_3+\text{CH}_2\text{O}=\text{CH}_4+\text{HCO}$ | 9.2(-21) | 2.81 | -2950 |
| 90. | $\text{CH}_3+\text{HCO}=\text{CH}_4+\text{CO}$ | 2.0(-10) | 0 | 0 |
| 91. | $\text{CH}_3+\text{H}_2\text{O}_2=\text{CH}_4+\text{HO}_2$ | 6.18(-14) | 0 | -645 |
| 92. | $\text{CH}_4+\text{O}=\text{CH}_3+\text{OH}$ | 3.55(-18) | 2.2 | -3266 |
| 93. | $\text{CH}_4+\text{OH}=\text{H}_2\text{O}+\text{CH}_3$ | 2.4(-12) | 0 | -1710 |

| 1 | 2 | 3 | 4 | 5 |
|------|---|-----------|------|--------|
| 94. | H+CO+M=HCO+M | 1.38(-36) | 1 | -781 |
| 95. | HCO+O ₂ =HO ₂ +CO | 5.02(-12) | 0 | 0 |
| 96. | HCO+H=H ₂ +CO | 2.0(-10) | 0 | 0 |
| 97. | HCO+O=OH+CO | 1.66(-10) | 0 | 0 |
| 98. | HCO+OH=H ₂ O+CO | 5.25(-11) | 0 | 0 |
| 99. | HCO+HO ₂ =CH ₂ O+O ₂ | 1.66(-10) | 0 | -1512 |
| 100. | HCO+H ₂ O ₂ =CH ₂ O+HO ₂ | 3.64(-14) | 0 | -3321 |
| 101. | 2HCO=CH ₂ O+CO | 3.00(-11) | 0 | 0 |
| 102. | 2HCO=H ₂ +2CO | 5.00(-12) | 0 | 0 |
| 103. | HCO+H+M=CH ₂ O+M | 3.89(-37) | 1 | 5947 |
| 104. | CH ₂ O+O=HCO+OH | 8.32(-11) | 0 | -2318 |
| 105. | CH ₂ O+H=HCO+H ₂ | 8.32(-11) | 0 | -2016 |
| 106. | CH ₂ O+OH=H ₂ O+HCO | 1.6(-11) | 0 | -110 |
| 107. | CH ₂ O+HO ₂ =H ₂ O ₂ +HCO | 3.32(-13) | 0 | -4032 |
| 108. | CH ₃ O+H=CH ₂ O+H ₂ | 3.30(-11) | 0 | 0 |
| 109. | CH ₃ O+O=CH ₂ O+OH | 1.00(-11) | 0 | 0 |
| 110. | CH ₃ O+OH=CH ₂ O+H ₂ O | 3.00(-11) | 0 | 0 |
| 111. | CH ₃ O+HO ₂ =CH ₂ O+H ₂ O ₂ | 5.00(-13) | 0 | 0 |
| 112. | CH ₃ O+O ₂ =CH ₂ O+HO ₂ | 1.1(-12) | 0 | -1310 |
| 113. | CH ₃ O+CH ₃ =CH ₂ O+CH ₄ | 4.01(-11) | 0 | 0 |
| 114. | CO+O+M=CO ₂ +M | 4.35(-25) | 0 | -2066 |
| 115. | OH+CO=H+CO ₂ | 1.5(-13) | 0 | 0 |
| 116. | HCO+O=H+CO ₂ | 5.0(-11) | 0 | 0 |
| 117. | CH ₃ O+CO=CH ₃ +CO ₂ | 2.61(-11) | 0 | -5940 |
| 118. | CH ₃ +O ₂ +M=CH ₃ O ₂ +M, M=O ₂ | 5.4(-26) | -2 | 0 |
| 119. | CH ₃ +O ₂ +M=CH ₃ O ₂ +M, M=N ₂ | 5.4(-26) | -2 | 0 |
| 120. | CH ₃ +OH+M=CH ₃ OH+M | 4.0(-35) | 1 | 5494 |
| 121. | CH ₂ O+H+M=CH ₂ OH+M | 1.35(-31) | -0.7 | -3820 |
| 122. | CH ₂ O+NO ₃ =HNO ₃ +HCO | 6(-16) | 0 | 0 |
| 123. | CH ₃ O+CH ₄ =CH ₃ OH+CH ₃ | 2.61(-13) | 0 | -4450 |
| 124. | CH ₃ O+CH ₂ O=CH ₃ OH+HCO | 1.69(-13) | 0 | -1500 |
| 125. | CH ₃ O+HCO=CH ₃ OH+CO | 1.5(-10) | 0 | 0 |
| 126. | CH ₃ O+NO ₂ =CH ₂ O+HNO ₂ | 3(-13) | 0 | 0 |
| 127. | CH ₃ O+NO ₂ +M=CH ₃ NO ₃ +M | 3.65(-18) | -4.5 | 0 |
| 128. | CH ₂ OH+O ₂ =CH ₂ O+HO ₂ | 2(-12) | 0 | 0 |
| 129. | CH ₃ OH+O=CH ₂ OH+OH | 2.82(-12) | 0 | -1154 |
| 130. | CH ₃ OH+H=CH ₂ OH+H ₂ | 5.02(-11) | 0 | -3528 |
| 131. | CH ₃ OH+H=CH ₃ +H ₂ O | 8.72(-12) | 0 | -2691 |
| 132. | CH ₃ OH+OH=H ₂ O+CH ₂ OH | 7.55(-12) | 0 | -690 |
| 133. | CH ₃ OH+OH=H ₂ O+CH ₃ O | 1.55(-12) | 0 | -690 |
| 134. | CH ₃ OH+CH ₃ =CH ₂ OH+CH ₄ | 3.02(-13) | 0 | -4939 |
| 135. | CH ₃ O ₂ +M=CH ₃ +O ₂ +M | 1.2(25) | -10 | -16731 |
| 136. | CH ₃ O ₂ +OH=CH ₃ OH+O ₂ | 1.0(-10) | 0 | 0 |
| 137. | CH ₃ O ₂ +H=CH ₃ O+OH | 1.6(-10) | 0 | 0 |
| 138. | CH ₃ O ₂ +O=CH ₃ O+O ₂ | 6.0(-11) | 0 | 0 |
| 139. | CH ₃ O ₂ +O ₃ =CH ₃ O+2O ₂ | 2(-17) | 0 | 0 |
| 140. | CH ₃ O ₂ +HO ₂ =CH ₃ O ₂ H+O ₂ | 7.71(-14) | 0 | 1300 |
| 141. | CH ₃ O ₂ +H ₂ O ₂ =CH ₃ O ₂ H+HO ₂ | 4.0(-12) | 0 | -5000 |
| 142. | CH ₃ O ₂ +CH ₂ O=CH ₃ O ₂ H+HCO | 3.3(-12) | 0 | -5870 |
| 143. | CH ₃ O ₂ +HCO=CH ₃ O+H+CO ₂ | 5.0(-11) | 0 | 0 |
| 144. | CH ₃ O ₂ +CH ₃ =2CH ₃ O | 4.0(-11) | 0 | 0 |
| 145. | CH ₃ O ₂ +NO=CH ₃ O+NO ₂ | 4.2(-12) | 0 | 180 |

| 1 | 2 | 3 | 4 | 5 |
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| 146. | $2\text{CH}_3\text{O}_2=\text{CH}_3\text{OH}+\text{CH}_2\text{O}+\text{O}_2$ | 2.1(-13) | 0 | 0 |
| 147. | $2\text{CH}_3\text{O}_2=2\text{CH}_3\text{O}+\text{O}_2$ | 1.3(-13) | 0 | 0 |
| 148. | $\text{CH}_3\text{O}+\text{CH}_3\text{O}_2=\text{CH}_2\text{O}+\text{CH}_3\text{O}_2\text{H}$ | 5.0(-13) | 0 | 0 |
| 149. | $\text{CH}_3\text{O}_2\text{H}+\text{OH}=\text{CH}_3\text{O}_2+\text{H}_2\text{O}$ | 5.38(-11) | 0 | -504 |
| 150. | $\text{CH}_3+\text{N}=\text{HCN}+2\text{H}$ | 1.18(-10) | 0 | 0 |
| Reactions with N, NO, CN, HCN, NCO | | | | |
| 151. | $\text{CN}+\text{O}=\text{CO}+\text{N}$ | 3.4(-12) | 0 | 0 |
| 152. | $\text{CN}+\text{O}_2=\text{CO}+\text{NO}$ | 1(-12) | 0 | 0 |
| 153. | $\text{CN}+\text{O}_2=\text{NCO}+\text{O}$ | 1.4(-11) | 0 | 0 |
| 154. | $\text{CN}+\text{OH}=\text{HCN}+\text{O}$ | 1.18(-11) | 0 | -1008 |
| 155. | $\text{CN}+\text{OH}=\text{NCO}+\text{H}$ | 9.33(-11) | 0 | 0 |
| 156. | $\text{CN}+\text{H}_2\text{O}=\text{HCN}+\text{OH}$ | 1.05(-11) | 0 | -3034 |
| 157. | $\text{CN}+\text{NO}_2=\text{NCO}+\text{NO}$ | 5.0(-11) | 0 | 0 |
| 158. | $\text{CN}+\text{N}_2\text{O}=\text{NCO}+\text{N}_2$ | 1.66(-11) | 0 | 0 |
| 159. | $\text{HCN}+\text{O}=\text{NCO}+\text{H}$ | 3.02(-16) | 1.5 | -3734 |
| 160. | $\text{HCN}+\text{OH}=\text{CN}+\text{H}_2\text{O}$ | 7.26(-12) | 0 | -4576 |
| 161. | $\text{NCO}+\text{O}=\text{NO}+\text{CO}$ | 9.55(-11) | 0 | 0 |
| 162. | $\text{NCO}+\text{O}=\text{CN}+\text{O}_2$ | 2.24(-11) | 0 | -2722 |
| 163. | $\text{NCO}+\text{H}=\text{NH}+\text{CO}$ | 6.61(-11) | 0 | 0 |
| 164. | $\text{NCO}+\text{H}=\text{HCN}+\text{O}$ | 8.32(-16) | 1.5 | -3931 |
| 165. | $\text{NCO}+\text{OH}=\text{NO}+\text{CO}+\text{H}$ | 1.66(-11) | 0 | 0 |
| 166. | $\text{NCO}+\text{N}=\text{N}_2+\text{CO}$ | 3.32(-11) | 0 | 0 |
| 167. | $\text{NCO}+\text{NO}=\text{N}_2\text{O}+\text{CO}$ | 1.66(-11) | 0 | 242 |
| 168. | $\text{N}+\text{CO}_2=\text{NO}+\text{CO}$ | 3.16(-13) | 0 | -1714 |
| 169. | $\text{CH}_3\text{O}+\text{NO}+\text{M}=\text{CH}_3\text{NO}_2+\text{M}, \text{M}=\text{N}_2$ | 6(-28) | 0 | 0 |
| Reactions with Cl, ClO, ClO ₂ , HCl, ClNO ₃ , CH ₃ Cl | | | | |
| 170. | $\text{Cl}+\text{O}_2+\text{M}=\text{ClO}_2+\text{M}, \text{M}=\text{N}_2$ | 1.7(-33) | 0 | 0 |
| 171. | $\text{ClO}_2+\text{M}=\text{Cl}+\text{O}_2+\text{M}, \text{M}=\text{N}_2$ | 1.5(-8) | 0 | -3285 |
| 172. | $\text{Cl}+\text{H}_2=\text{HCl}+\text{H}$ | 3.7(-11) | 0 | -2300 |
| 173. | $\text{Cl}+\text{HO}_2=\text{HCl}+\text{O}_2$ | 1.8(-11) | 0 | 170 |
| 174. | $\text{Cl}+\text{HO}_2=\text{ClO}+\text{OH}$ | 4.1(-11) | 0 | -450 |
| 175. | $\text{Cl}+\text{H}_2\text{O}_2=\text{HCl}+\text{HO}_2$ | 1.1(-11) | 0 | -980 |
| 176. | $\text{Cl}+\text{O}_3=\text{ClO}+\text{O}_2$ | 2.7(-11) | 0 | -257 |
| 177. | $\text{Cl}+\text{CH}_4=\text{HCl}+\text{CH}_3$ | 9.6(-12) | 0 | -1350 |
| 178. | $\text{Cl}+\text{CH}_2\text{O}=\text{HCl}+\text{HCO}$ | 8.2(-11) | 0 | -34 |
| 179. | $\text{Cl}+\text{NO}_3=\text{ClO}+\text{NO}_2$ | 2.6(-11) | 0 | 0 |
| 180. | $\text{Cl}+\text{HNO}_3=\text{HCl}+\text{NO}_3$ | 1.7(-14) | 0 | 0 |
| 181. | $\text{Cl}+\text{CH}_3\text{Cl}=\text{HCl}+\text{CH}_2\text{Cl}$ | 3.4(-11) | 0 | -1260 |
| 182. | $\text{Cl}+\text{ClO}_2=2\text{ClO}$ | 3.4(-11) | 0 | 160 |
| 183. | $\text{Cl}+\text{ClNO}_3=\text{Cl}_2+\text{NO}_3$ | 6.8(-12) | 0 | 160 |
| 184. | $\text{ClO}+\text{HO}_2=\text{HCl}+\text{O}_3$ | 2(-14) | 0 | 0 |
| 185. | $\text{ClO}+\text{HO}_2=\text{HOCl}+\text{O}_2$ | 4.6(-13) | 0 | 710 |
| 186. | $\text{ClO}+\text{NO}=\text{Cl}+\text{NO}_2$ | 6.2(-12) | 0 | 294 |
| 187. | $\text{ClO}+\text{NO}_2+\text{M}=\text{ClNO}_3+\text{M}, \text{M}=\text{O}_2$ | 4.49(-23) | -3.4 | 0 |
| 188. | $\text{ClO}+\text{NO}_2+\text{M}=\text{ClNO}_3+\text{M}, \text{M}=\text{N}_2$ | 4.49(-23) | -3.4 | 0 |
| 189. | $\text{O}+\text{HCl}=\text{OH}+\text{Cl}$ | 1(-11) | 0 | -3340 |
| 190. | $\text{O}+\text{HOCl}=\text{OH}+\text{ClO}$ | 1(-11) | 0 | -2200 |
| 191. | $\text{O}+\text{ClO}=\text{O}_2+\text{Cl}$ | 6.4(-11) | 0 | -120 |
| 192. | $\text{O}+\text{ClNO}_3=\text{ClO}_2+\text{NO}_2$ | 1.9(-13) | 0 | 0 |
| 193. | $\text{OH}+\text{HCl}=\text{H}_2\text{O}+\text{Cl}$ | 2.8(-12) | 0 | -425 |
| 194. | $\text{OH}+\text{HOCl}=\text{H}_2\text{O}+\text{ClO}$ | 3(-12) | 0 | -500 |
| 195. | $\text{OH}+\text{ClO}=\text{HO}_2+\text{Cl}$ | 9.46(-12) | 0 | 120 |

| 1 | 2 | 3 | 4 | 5 |
|---|---|-----------|------|-------|
| 196. | OH+ClO=HCl+O ₂ | 1.54(-12) | 0 | 120 |
| 197. | OH+CH ₃ Cl=H ₂ O+CH ₂ Cl | 1.9(-12) | 0 | -1120 |
| 198. | O+ClNO ₃ =ClO ₂ +NO ₂ | 1.9(-13) | 0 | 0 |
| 199. | OH+ClNO ₃ =HNO ₃ +ClO | 0 | 0 | 0 |
| 200. | OH+ClNO ₃ =HOCl+NO ₃ | 1.2(-12) | 0 | -330 |
| Reactions with CFCl ₃ , CF ₂ Cl ₂ | | | | |
| 201. | OH+CFCl ₃ =HOCl+CFCl ₂ | 1(-12) | 0 | -3650 |
| 202. | OH+CF ₂ Cl ₂ =HOCl+CF ₂ Cl | 1(-12) | 0 | -3540 |
| Reactions with SO ₂ , SO ₃ , HSO ₃ | | | | |
| 203. | O+SO ₂ +M=SO ₃ +M, M=O ₂ | 4.0(-32) | 0 | -1000 |
| 204. | O+SO ₂ +M=SO ₃ +M, M=N ₂ | 4.0(-32) | 0 | -1000 |
| 205. | OH+SO ₂ +M=HSO ₃ +M, M=O ₂ | 4.58(-24) | -2.9 | 0 |
| 206. | OH+SO ₂ +M=HSO ₃ +M, M=N ₂ | 4.58(-24) | -2.9 | 0 |
| 207. | HO ₂ +SO ₂ =PRODUCTS | 1.1(-18) | 0 | 0 |
| 208. | CH ₃ O ₂ +SO ₂ =CH ₃ O+SO ₃ | 5(-17) | 0 | 0 |
| 209. | HSO ₃ +O ₂ =HO ₂ +SO ₃ | 4(-13) | 0 | 0 |
| 210. | SO ₃ +H ₂ O=H ₂ SO ₄ | 1.2(-15) | 0 | 0 |
| Reactions with O(¹ D) | | | | |
| 211. | O(¹ D)+M=O+M, M=O ₂ | 4.2(-11) | 0 | 0 |
| 212. | O(¹ D)+M=O+M, M=N ₂ | 2.6(-11) | 0 | 0 |
| 213. | O(¹ D)+M=O+M, M=H ₂ O | 1.2(-11) | 0 | 0 |
| 214. | O(¹ D)+M=O+M, M=H ₂ | 1.2(-11) | 0 | 0 |
| 215. | O(¹ D)+O+M=O ₂ +M | 1(-32) | 0 | 0 |
| 216. | 2O(¹ D)+M=O ₂ +M | 5(-33) | 0 | 0 |
| 217. | O(¹ D)+O ₃ =O ₂ + ₂ O | 1.2(-10) | 0 | 0 |
| 218. | O(¹ D)+O ₃ =2O ₂ | 1.2(-10) | 0 | 0 |
| 219. | O(¹ D)+H ₂ =OH+H | 1.1(-10) | 0 | 0 |
| 220. | O(¹ D)+H ₂ O= ₂ OH | 2.3(-10) | 0 | 0 |
| 221. | O(¹ D)+H ₂ O=H ₂ +O ₂ | 2.3(-12) | 0 | 0 |
| 222. | O(¹ D)+N ₂ O=N ₂ +O ₂ | 4.4(-11) | 0 | 0 |
| 223. | O(¹ D)+N ₂ O=2NO | 7.2(-11) | 0 | 0 |
| 224. | O(¹ D)+CH ₄ =OH+CH ₃ | 1.4(-10) | 0 | 0 |
| 225. | O(¹ D)+CH ₄ =CH ₂ O+H ₂ | 1.5(-11) | 0 | 0 |
| 226. | O(¹ D)+F ₂ CO=CO ₂ +F ₂ | 2.2(-11) | 0 | 0 |
| 227. | O(¹ D)+CF ₂ Cl ₂ =ClO+CF ₂ Cl | 7.7(-11) | 0 | 0 |
| 228. | O(¹ D)+CF ₂ Cl ₂ =O+CF ₂ Cl ₂ | 2.1(-11) | 0 | 0 |
| 229. | O(¹ D)+CF ₂ Cl ₂ =F ₂ CO+Cl ₂ | 2.1(-11) | 0 | 0 |
| 230. | O(¹ D)+CF ₂ Cl ₂ =FCICO+ClF | 2.1(-11) | 0 | 0 |
| 231. | O(¹ D)+CFCl ₃ =ClO+CFCl ₂ | 1.38(-10) | 0 | 0 |
| 232. | O(¹ D)+CFCl ₃ =O+CFCl ₃ | 3.68(-11) | 0 | 0 |
| 233. | O(¹ D)+CFCl ₃ =FCICO+Cl ₂ | 2.76(-11) | 0 | 0 |
| 234. | O(¹ D)+CFCl ₃ =Cl ₂ CO+ClF | 2.76(-11) | 0 | 0 |
| 235. | O(¹ D)+CCl ₄ =ClO+CCl ₃ | 2.84(-10) | 0 | 0 |
| 236. | O(¹ D)+CCl ₄ =O+CCl ₄ | 4.6(-11) | 0 | 0 |
| 237. | O(¹ D)+CCl ₄ =Cl ₂ CO+Cl ₂ | 0 | 0 | 0 |

A(-n) corresponds A·10⁻ⁿ

Table 7. Photochemical reactions list for plume chemistry model.

| № | Reactions | Rate I (s^{-1}) | |
|-----|---------------------------|-----------------------|-----------|
| | | $H=10$ km | $H=20$ km |
| 1. | $O_2+h\nu=2O$ | 6.85(-18) | 9.39(-13) |
| 2. | $O_2+h\nu=O+O(^1D)$ | 0 | 0 |
| 3. | $O_3+h\nu=O_2+O(^1D)$ | 1.44(-8) | 1.96(-5) |
| 4. | $O_3+h\nu=O_2+O$ | 3.06(-4) | 4.042(-4) |
| 5. | $H_2O+h\nu=H+OH$ | 3.71(-18) | 1.77(-12) |
| 6. | $H_2O_2+h\nu=2OH$ | 7.21(-6) | 7.74(-6) |
| 7. | $HO_2+h\nu=O+OH$ | 4.13(-12) | 5.38(-7) |
| 8. | $H_2O+h\nu=H_2+O(^1D)$ | 5.08(-15) | 2.42(-9) |
| 9. | $NO+h\nu=N+O$ | 2.27(-14) | 4.12(-11) |
| 10. | $NO_2+h\nu=NO+O$ | 6.51(-3) | 6.55(-3) |
| 11. | $NO_3+h\nu=NO_2+O$ | 2.2(-2) | 2.2(-2) |
| 12. | $NO_3+h\nu=NO+O_2$ | 0 | 0 |
| 13. | $N_2O_5+h\nu=NO_2+NO_3$ | 3.03(-5) | 3.23(-5) |
| 14. | $HNO_2+h\nu=OH+NO$ | 6.6(-4) | 6.6(-4) |
| 15. | $HNO_3+h\nu=NO_2+OH$ | 4.61(-7) | 7.88(-7) |
| 16. | $HNO_4+h\nu=NO_3+OH$ | 5.6(-6) | 6.71(-6) |
| 17. | $CO_2+h\nu=CO+O$ | 1.92(-18) | 2.99(-13) |
| 18. | $CH_4+h\nu=H+CH_3$ | 0 | 0 |
| 19. | $CH_2O+h\nu=H+HCO$ | 3.16(-5) | 3.43(-5) |
| 20. | $CH_2O+h\nu=H_2+CO$ | 5.8(-5) | 5.95(-5) |
| 21. | $Cl_2+h\nu=2Cl$ | 2.12(-3) | 2.15(-3) |
| 22. | $ClO+h\nu=Cl+O$ | 2.1(-5) | 3.76(-5) |
| 23. | $HCl+h\nu=H+Cl$ | 3.97(-15) | 8.53(-10) |
| 24. | $HOCl+h\nu=OH+Cl$ | 2.72(-4) | 2.30(-4) |
| 25. | $CFCl_3+h\nu=CFCl_2+Cl$ | 0 | 0 |
| 26. | $CF_2Cl_2+h\nu=CF_2Cl+Cl$ | 0 | 0 |
| 27. | $CCl_4+h\nu=CCl_3+Cl$ | 2.84(-15) | 4.14(-8) |
| 28. | $CH_3Cl+h\nu=CH_3+Cl$ | 2.34(-15) | 5.41(-10) |

A(-n) corresponds $A \cdot 10^{-n}$

Table 8. The variation of the temperature and gas composition at the variations planes of the plume for B-747 aircraft for flight regime $M_\infty=0.8$; $H=10.7$ km

| x, m | atmosphere | 0 | 1 | 10 | 100 | 1000 |
|---------------------------------|------------|------------|------------|------------|------------|------------|
| T, K | 218.5 | 590 | 590 | 589.87 | 247.26 | 220.59 |
| H ₂ O | 5.768(-5) | 4.001(-2) | 4.001(-2) | 4.001(-2) | 4.094(-3) | 2.758(-4) |
| O ₂ | 2.002(-1) | 1.540(-1) | 1.540(-1) | 1.540(-1) | 1.955(-1) | 1.999(-1) |
| H ₂ | 9.378(-7) | 1.470(-6) | 1.470(-6) | 1.470(-6) | 9.916(-7) | 9.407(-7) |
| OH | 1.070(-13) | 2.981(-7) | 1.015(-9) | 6.201(-19) | 3.299(-14) | 2.030(-14) |
| H | 2.350(-20) | 3.411(-11) | 3.674(-14) | 2.282(-23) | 4.253(-20) | 7.555(-21) |
| O | 1.664(-15) | 1.830(-8) | 8.167(-11) | 1.011(-20) | 6.475(-18) | 6.859(-19) |
| N ₂ | 7.995(-1) | 7.742(-1) | 7.742(-1) | 7.742(-1) | 7.969(-1) | 7.993(-1) |
| HO ₂ | 1.406(-11) | 7.262(-10) | 1.390(-11) | 4.607(-19) | 2.205(-14) | 1.574(-15) |
| H ₂ O ₂ | 8.793(-10) | 1.080(-6) | 1.079(-6) | 1.079(-6) | 1.098(-7) | 6.764(-9) |
| N | 4.228(-27) | 6.512(-21) | 0 | 0 | 7.205(-30) | 6.915(-30) |
| NO | 1.003(-11) | 1.040(-4) | 9.802(-5) | 9.796(-5) | 9.886(-6) | 5.301(-7) |
| NO ₂ | 6.027(-12) | 4.491(-5) | 5.707(-5) | 5.713(-5) | 5.781(-6) | 3.163(-7) |
| HNO ₂ | 3.879(-14) | 4.161(-5) | 4.140(-5) | 4.140(-5) | 4.182(-6) | 2.260(-7) |
| N ₂ O | 2.811(-7) | 2.781(-5) | 2.781(-5) | 2.781(-5) | 3.062(-6) | 4.314(-7) |
| HNO | 0 | 7.532(-15) | 1.399(-10) | 1.400(-10) | 1.417(-11) | 7.659(-13) |
| O ₃ | 7.275(-8) | 7.732(-8) | 6.872(-8) | 9.978(-9) | 5.637(-8) | 6.765(-8) |
| HNO ₃ | 2.271(-10) | 2.231(-7) | 2.593(-7) | 2.594(-7) | 2.642(-8) | 1.652(-9) |
| NO ₃ | 3.598(-15) | 5.982(-6) | 2.322(-11) | 3.347(-12) | 2.492(-13) | 1.055(-13) |
| N ₂ O ₅ | 1.653(-13) | 1.029(-18) | 1.137(-15) | 1.648(-16) | 1.121(-10) | 1.081(-10) |
| HNO ₄ | 1.061(-10) | 1.087(-23) | 2.240(-16) | 1.829(-21) | 9.125(-11) | 1.055(-10) |
| CH ₃ | 1.855(-21) | 5.671(-28) | 0 | 9.541(-24) | 1.566(-20) | 2.743(-21) |
| CH ₄ | 1.496(-6) | 2.731(-25) | 2.730(-25) | 5.314(-14) | 1.344(-6) | 1.487(-6) |
| CO | 2.283(-7) | 2.991(-6) | 2.991(-6) | 2.991(-6) | 5.073(-7) | 2.433(-7) |
| CO ₂ | 3.092(-4) | 3.151(-2) | 3.151(-2) | 3.151(-2) | 3.461(-3) | 4.795(-4) |
| CH ₂ O | 1.900(-11) | 4.871(-18) | 4.871(-18) | 5.558(-18) | 1.715(-11) | 1.924(-11) |
| CH ₃ O | 8.917(-18) | 4.671(-28) | 0 | 5.607(-23) | 4.636(-17) | 3.301(-17) |
| CH ₃ O ₂ | 2.710(-12) | 8.202(-26) | 0 | 5.383(-21) | 1.953(-14) | 1.823(-14) |
| CH ₃ NO ₂ | 0 | 0 | 7.307(-26) | 7.965(-20) | 2.260(-12) | 2.210(-12) |
| CH ₃ NO ₃ | 0 | 0 | 7.784(-29) | 1.240(-22) | 1.123(-13) | 2.547(-13) |
| SO ₂ | 0 | 6.912(-6) | 6.911(-6) | 6.911(-6) | 6.982(-7) | 3.772(-8) |
| SO ₃ | 0 | 1.539(-23) | 3.086(-10) | 1.859(-12) | 2.175(-14) | 1.836(-14) |
| HSO ₃ | 0 | 1.465(-21) | 7.134(-15) | 4.341(-24) | 1.795(-18) | 1.128(-19) |
| H ₂ SO ₄ | 0 | 0 | 1.879(-10) | 4.963(-10) | 5.049(-11) | 2.901(-12) |
| Cl | 2.316(-16) | 0 | 0 | 2.064(-20) | 4.610(-13) | 1.844(-13) |
| ClO | 6.578(-13) | 0 | 0 | 1.996(-21) | 3.040(-15) | 9.228(-15) |
| ClO ₂ | 0 | 0 | 0 | 2.748(-25) | 4.172(-14) | 9.536(-14) |
| ClNO ₃ | 3.407(-13) | 0 | 0 | 1.216(-20) | 3.416(-13) | 5.677(-13) |
| HCl | 1.934(-10) | 0 | 0 | 6.873(-18) | 1.739(-10) | 1.925(-10) |
| HOCl | 4.138(-12) | 0 | 0 | 1.470(-19) | 3.720(-12) | 4.115(-12) |
| CH ₂ Cl | 0 | 0 | 0 | 0 | 4.553(-17) | 2.400(-16) |
| CH ₃ Cl | 5.442(-10) | 0 | 0 | 1.934(-17) | 4.893(-10) | 5.413(-10) |
| Cl ₂ | 3.834(-18) | 0 | 0 | 1.362(-25) | 4.824(-18) | 3.011(-17) |
| CCl ₃ | 0 | 0 | 0 | 0 | 1.405(-21) | 1.218(-21) |
| CCl ₄ | 1.214(-10) | 0 | 0 | 4.315(-18) | 1.092(-10) | 1.208(-10) |
| CFCl ₂ | 0 | 0 | 0 | 0 | 4.058(-23) | 5.573(-24) |
| CFCl ₃ | 1.406(-10) | 0 | 0 | 4.994(-18) | 1.264(-10) | 1.398(-10) |
| CF ₂ Cl | 0 | 0 | 0 | 0 | 8.997(-23) | 1.407(-23) |
| CF ₂ Cl ₂ | 2.339(-10) | 0 | 0 | 8.311(-18) | 2.103(-10) | 2.326(-10) |

A(-n) corresponds A·10⁻ⁿ

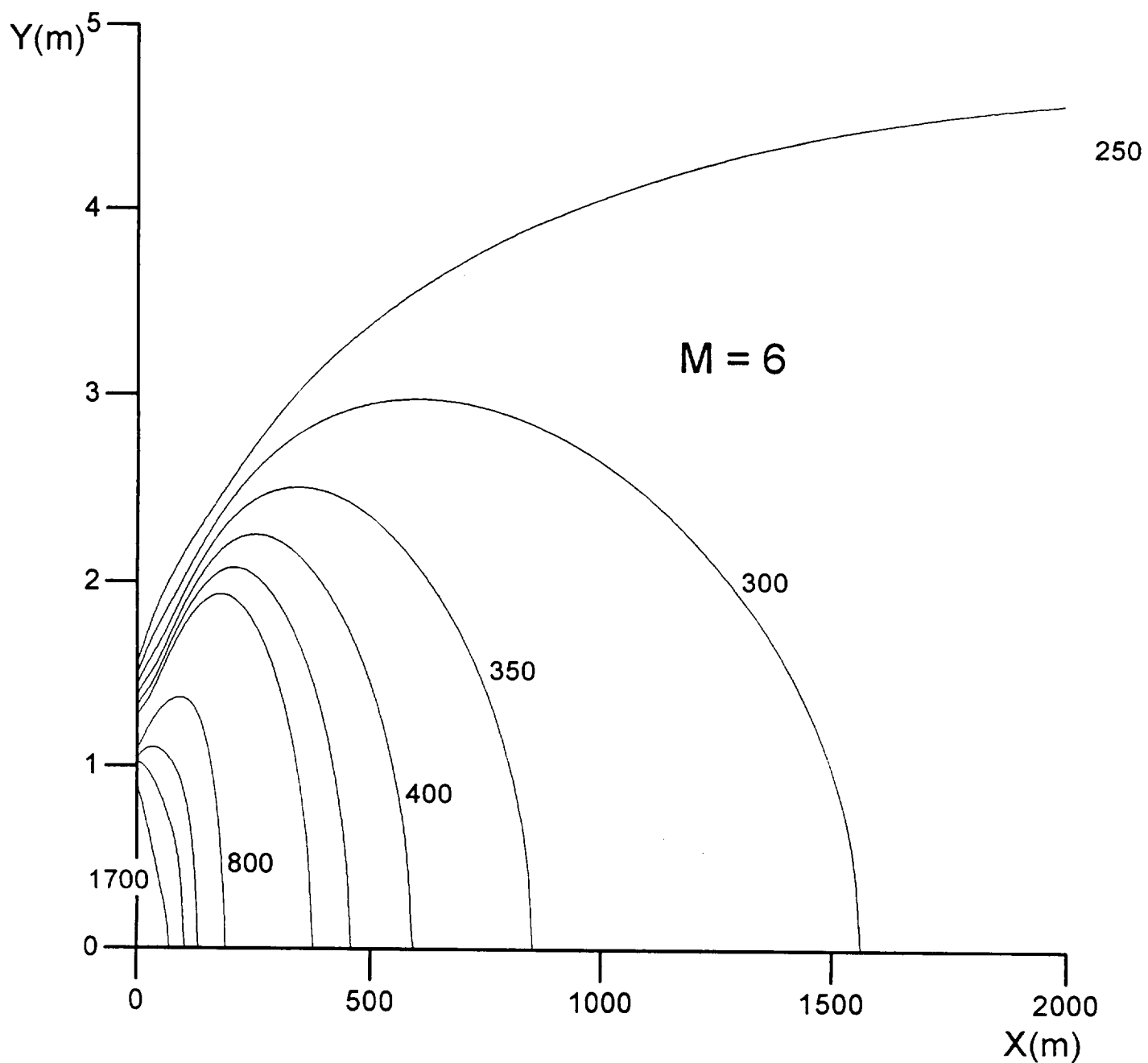


Fig. 1. The temperature field in the plume of hypersonic aircraft with hydrogen ramjet combustion engine for flight regime: $M_\infty=6$; $H=29$ km; $T_n=1800$ K; $P_n=P_\infty=13.9$ Pa; $T_\infty=225.5$ K.

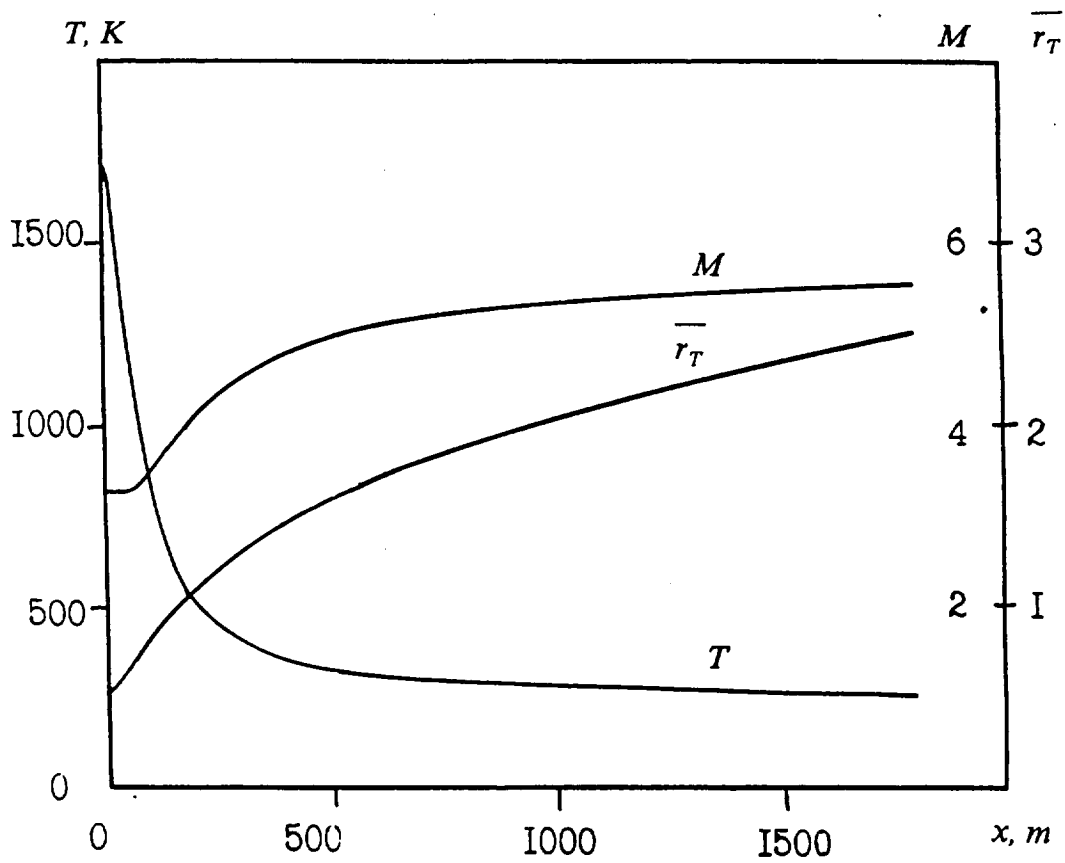


Fig. 2. Variation T , Mach number M , radius of the plume $\bar{r}_T = r_T/D_n$, $D_n=0.28 m$ along the plume for hypersonic aircraft with H_2 +air combustion engine for the following flight regime: $H=29 km$; $M_\infty=6$; $T_n=1800 K$; $P_n=P_\infty=13.9 Pa$.

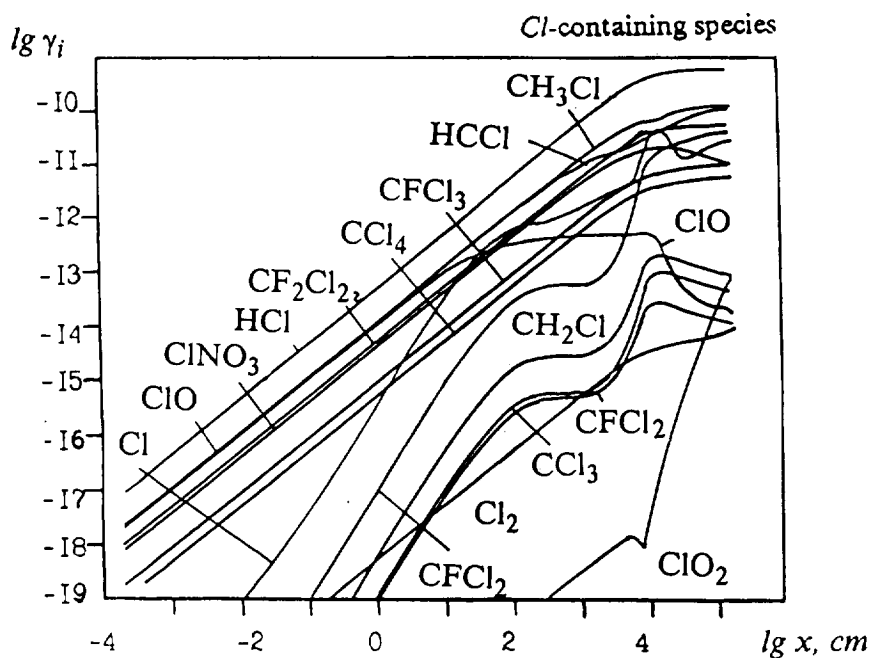
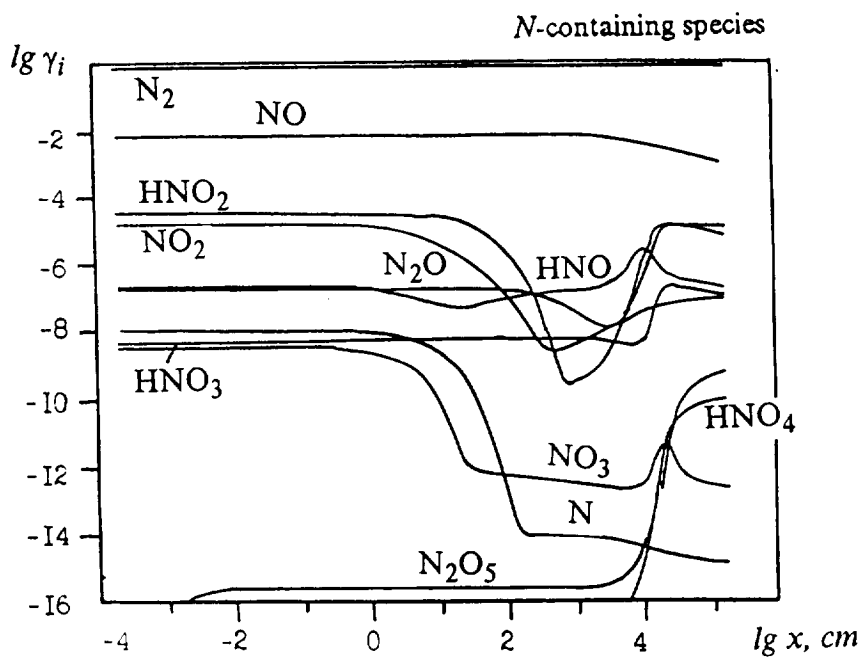
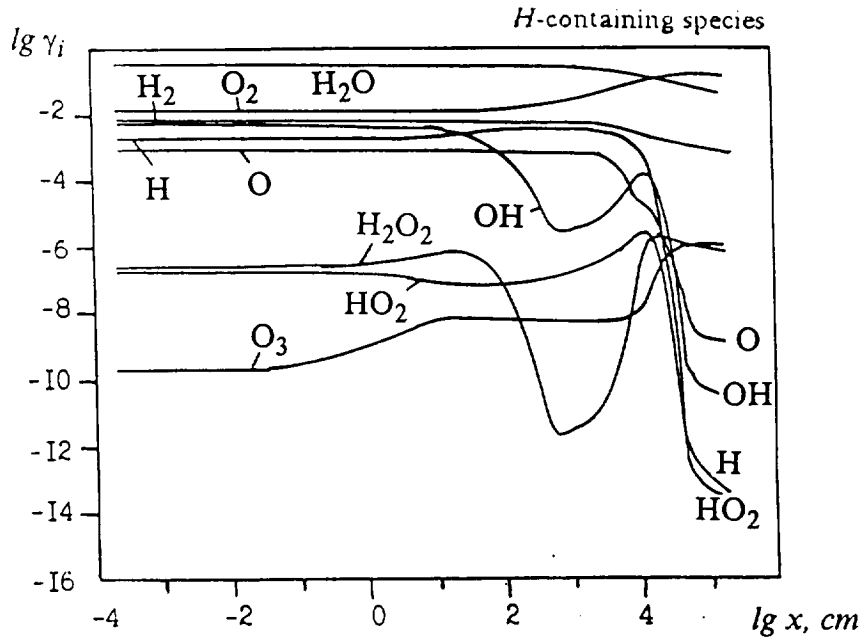


Fig. 3. The variation of mixture composition along the plume for the hypersonic aircraft with

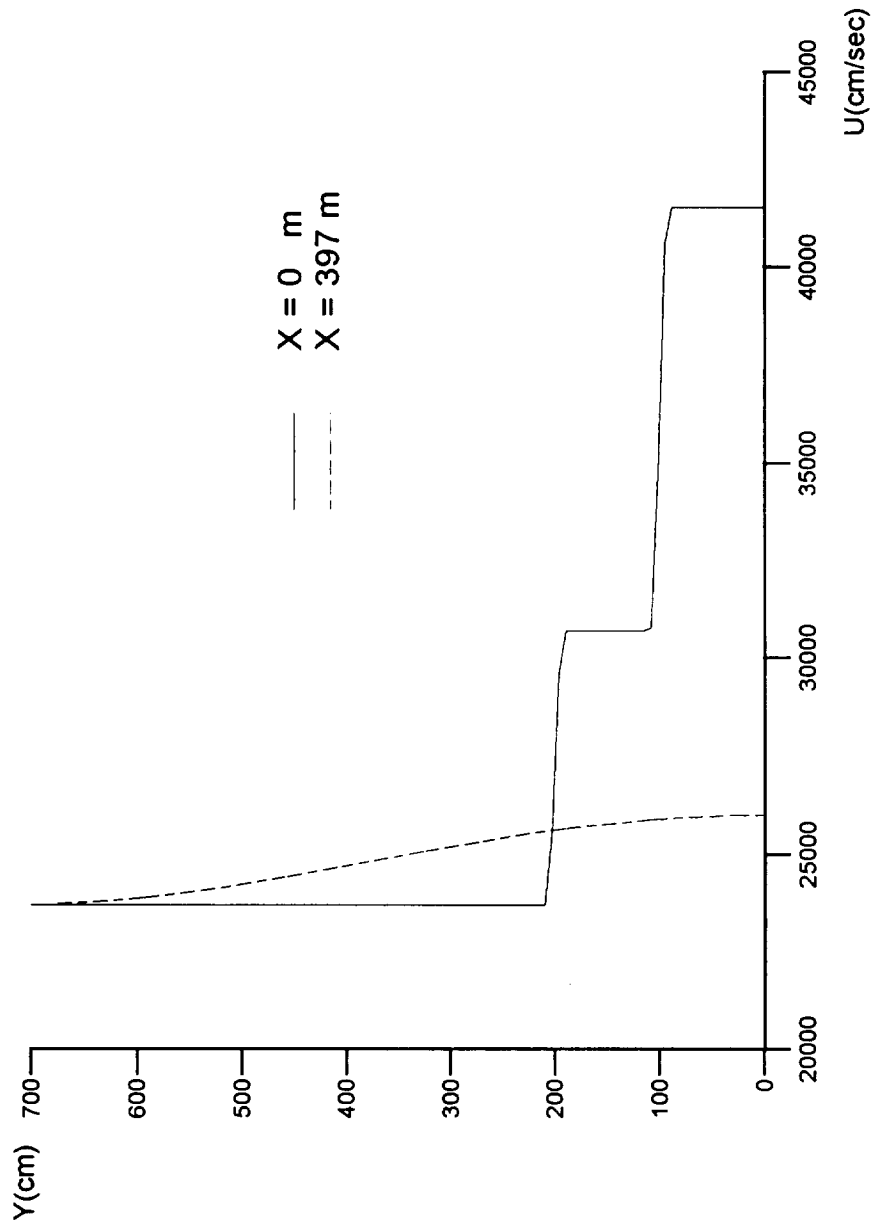


Fig. 4. Profiles of velocity across the plume $U=f(y)$ at the nozzle exit plane ($x=0$) and at the plane of plume corresponding $x=397$ m.

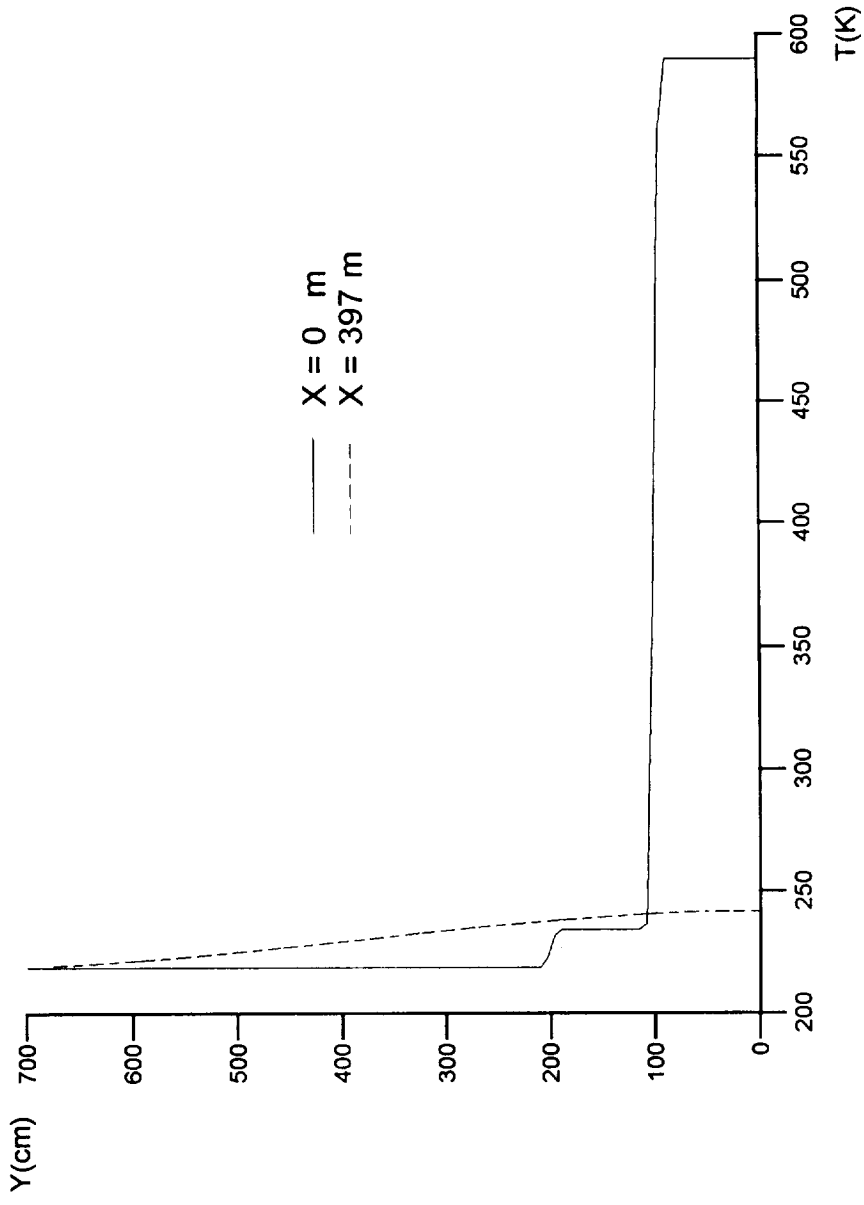


Fig. 5. Profiles of temperature across the plume $T=f(y)$ at the nozzle exit plane ($x=0$) and at the plane of plume corresponding $x=397$ m.

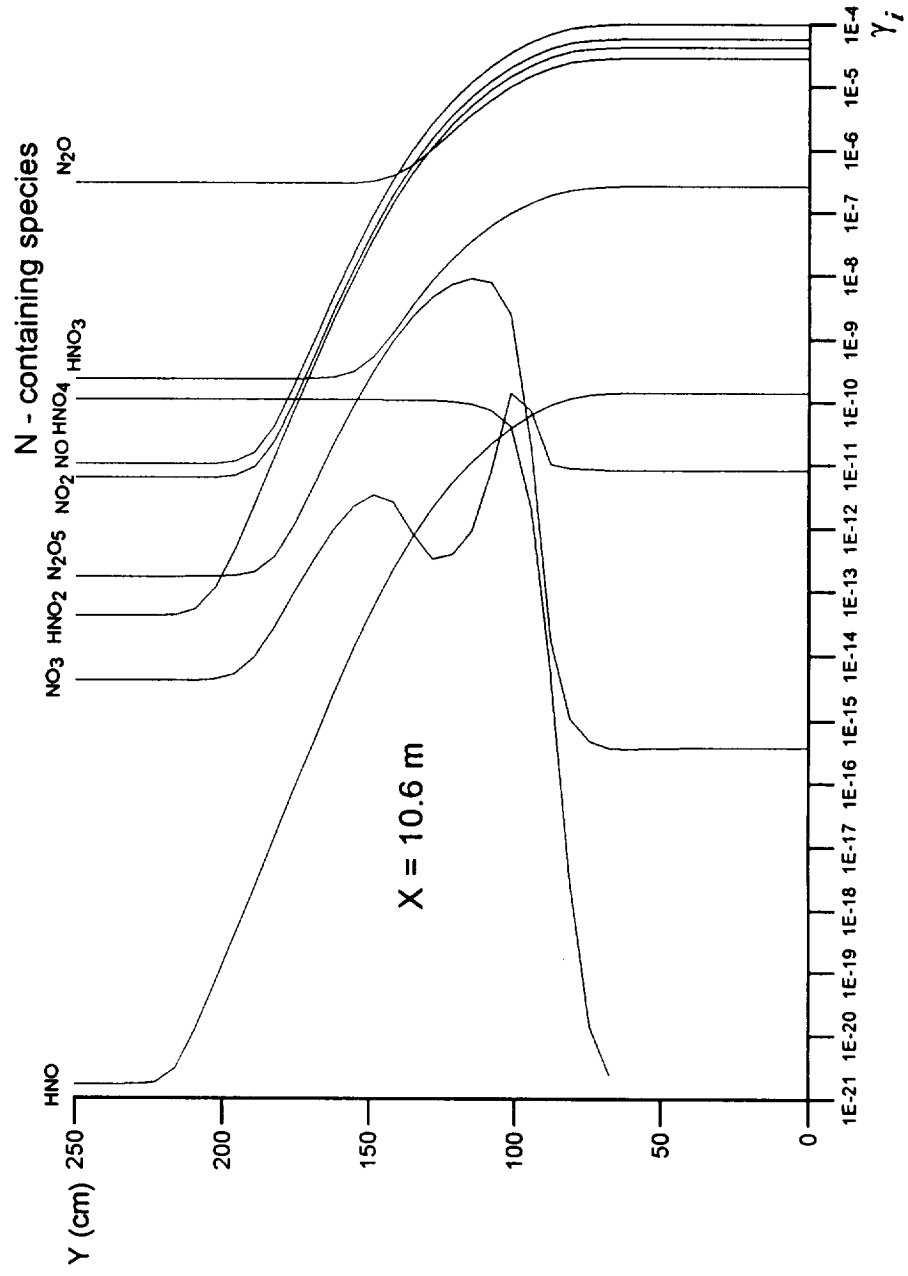


Fig. 6 a. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=10.6$ m.

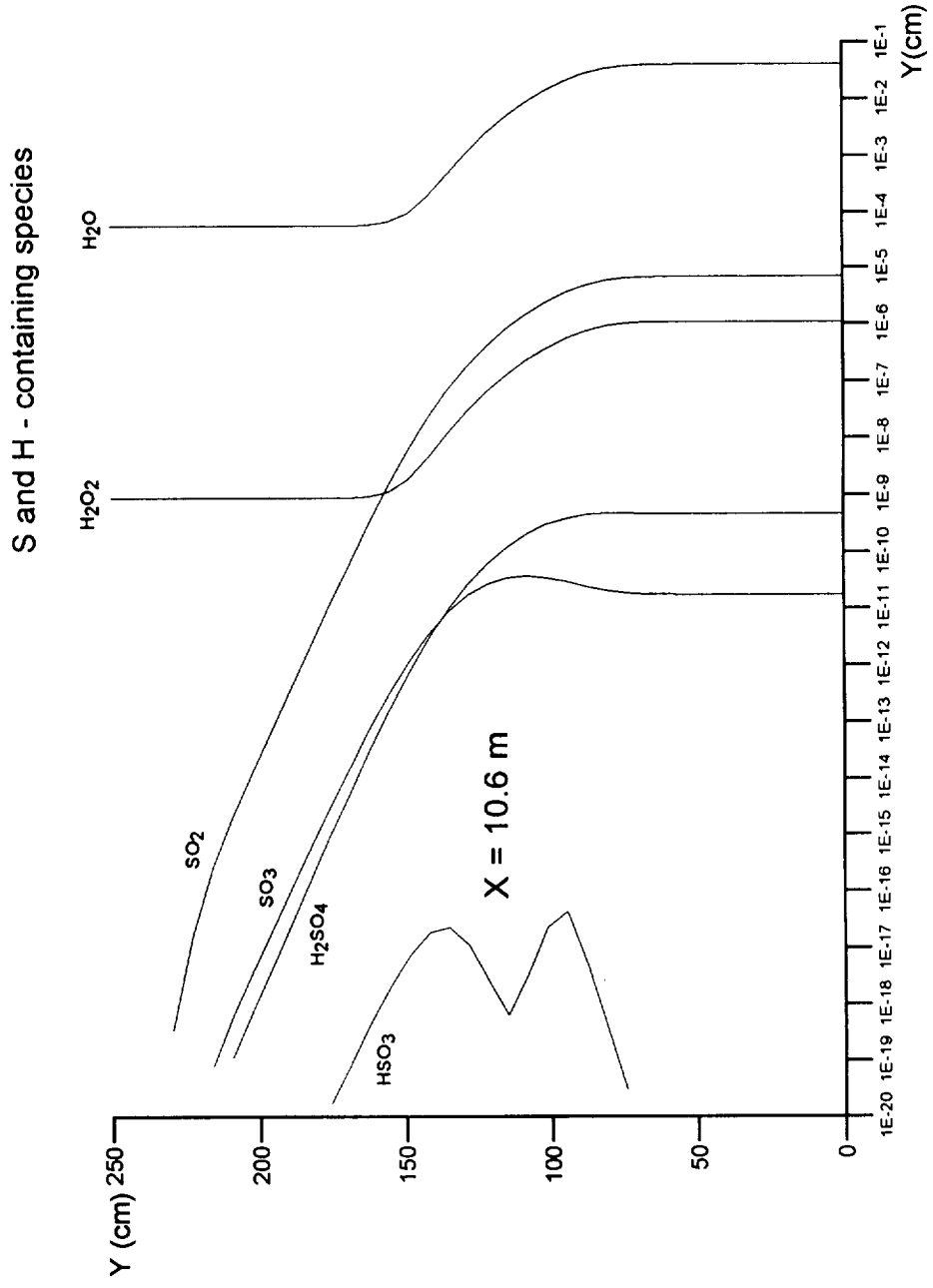


Fig. 6 b. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=10.6 \text{ m}$.

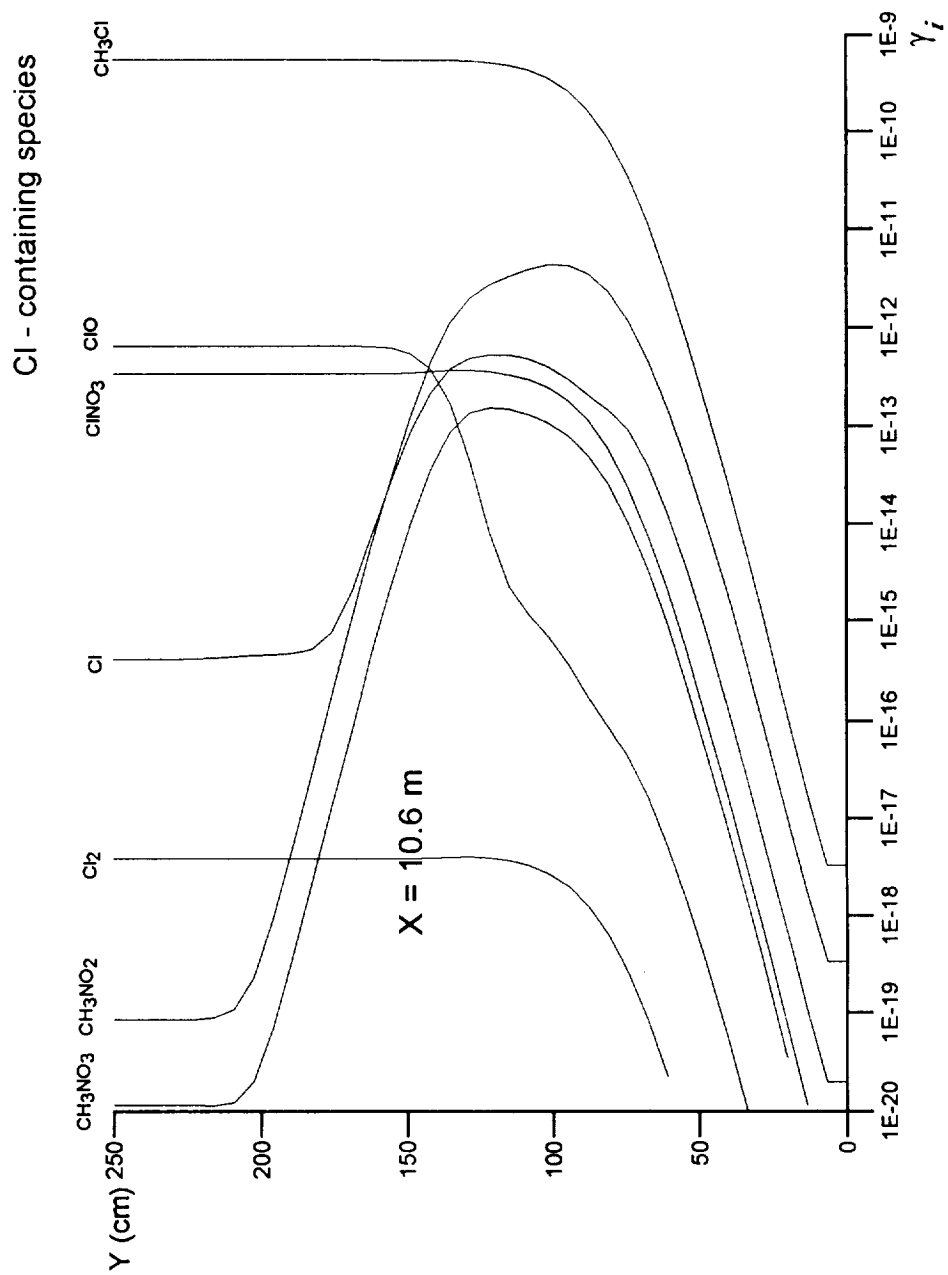


Fig. 6 c. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=10.6 \text{ m}$.

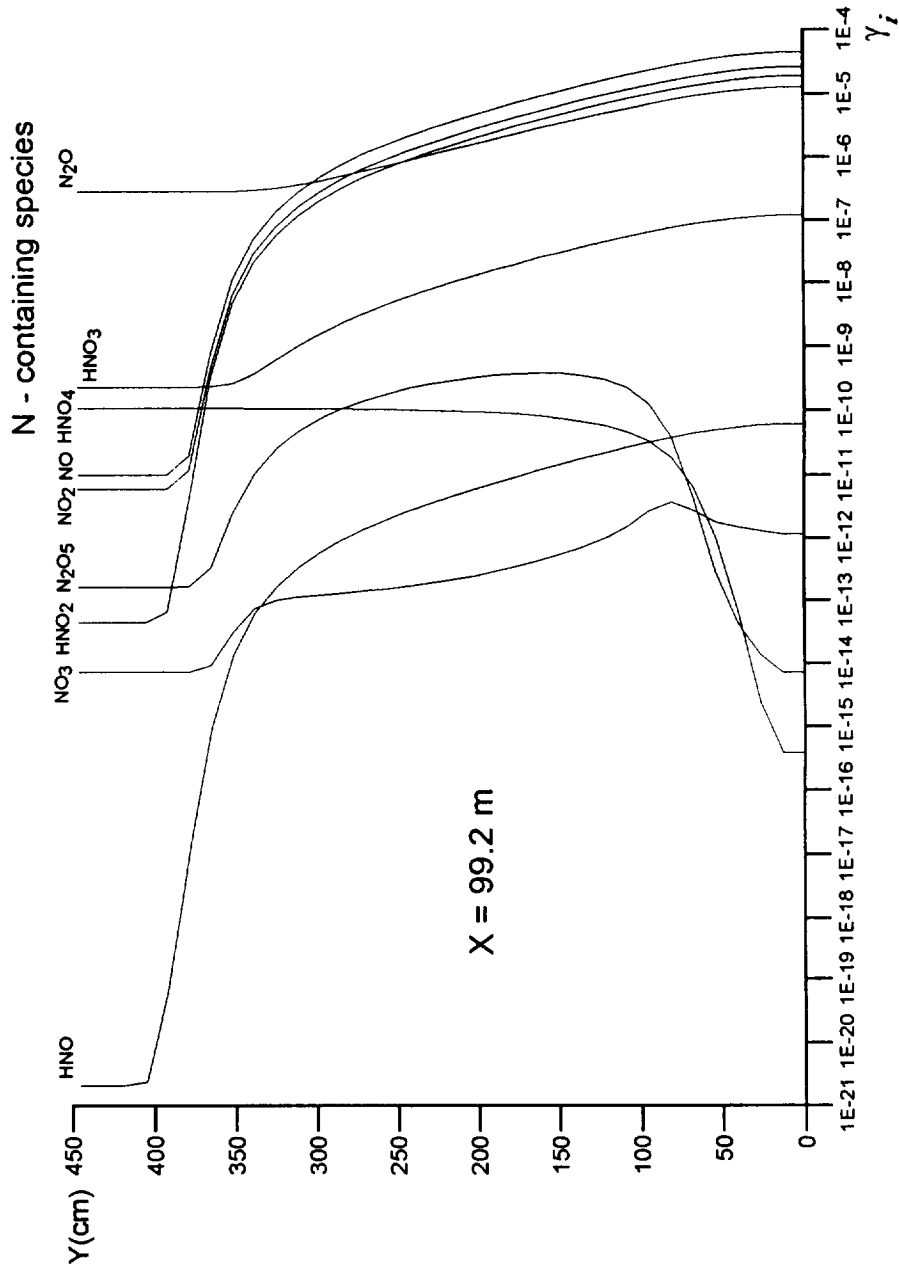


Fig. 7 a. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=99.2 \text{ m}$.

S and H - containing species

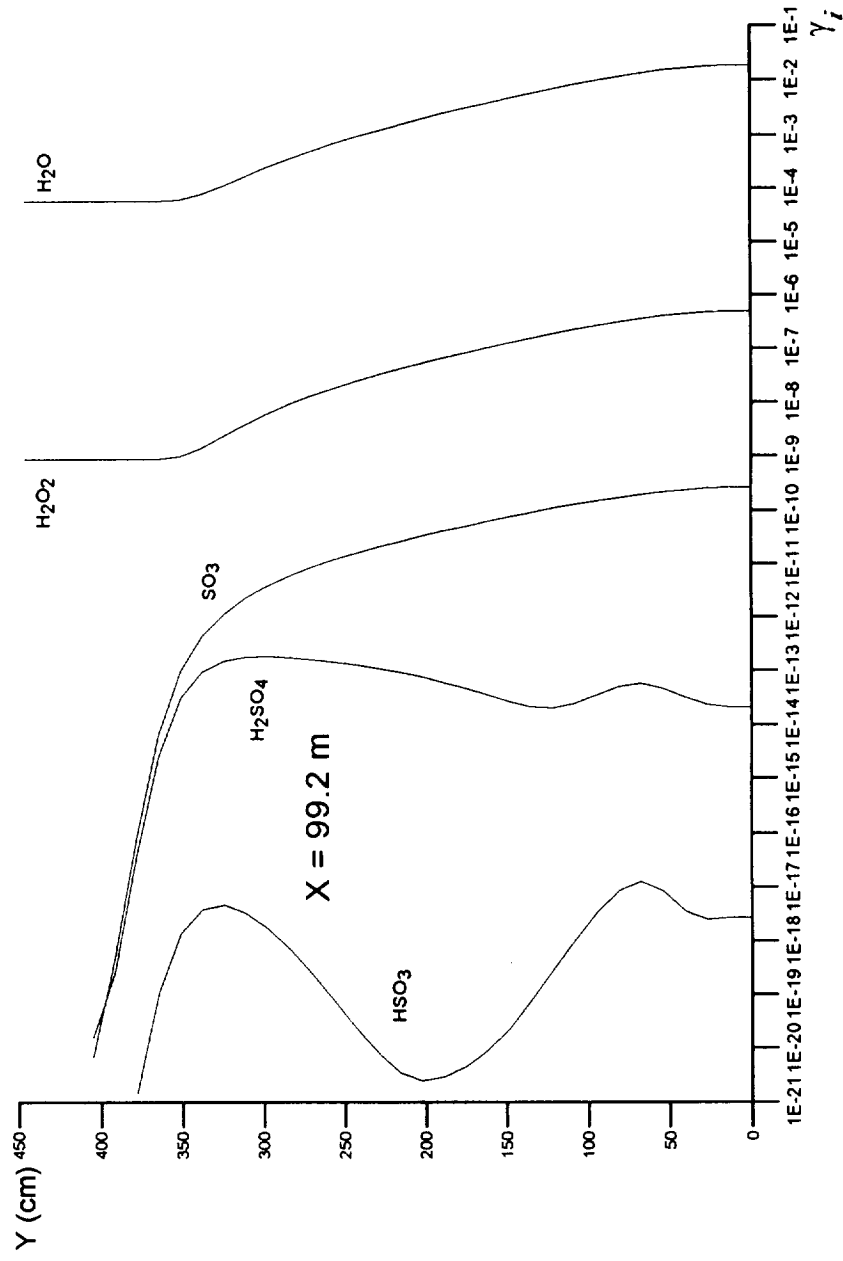


Fig. 7 b. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=99.2$ m.

Cl - containing species

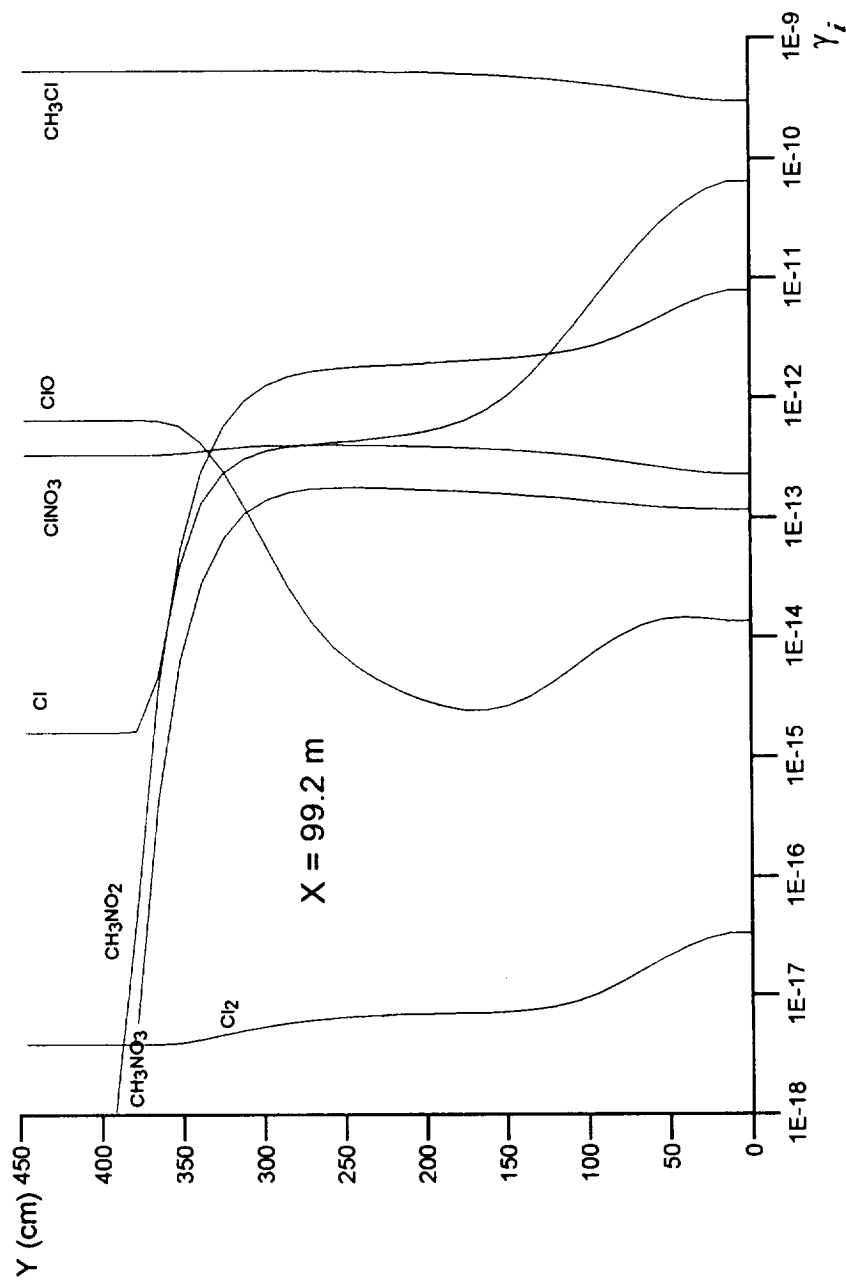


Fig. 7 c. Profiles of component concentrations (in mole fraction) across the plume at the plane of plume corresponding $x=99.2$ m.