

APPLICATION OF INTEGRATED CHEMICAL KINETIC MECHANISM REDUCTION SCHEME ON SMALL- SCALE MECHANISM - ETHYLENE

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Abstract

This work is an extension to a formerly reported work on development of integrated chemical kinetic mechanism reduction scheme to produce compact mechanisms for computational fluid dynamics (CFD) simulations. Upon successful application on large-scale mechanisms in the previous work, the reduction scheme is employed here to investigate its applicability on small-scale mechanism using a 111-species detailed ethylene model. The final reduced model consists of 27 species with 147 elementary reactions, and it is 75.7% smaller than the detailed model in terms of total number of species. The reduced model is then applied in one-dimensional laminar flame-speed simulations for model validations. The flame temperature profile computed by the detailed model is successfully replicated by the reduced model, with a maximum deviation of 2.8%. Subsequently, the fidelity of the reduced model is further assessed in zero-dimensional chemical kinetic simulations under a wide range of shock tube and jet stirred reactor (JSR) conditions. The simulation results show that the reduced model is able to reproduce the species concentration profiles and kinetics of the fuel oxidation adequately in view of its simplified fuel chemistry. The maximum relative error between the computations of the detailed and reduced models is recorded at 20%. In addition, the reduced model is also validated against the experimental results of ethylene oxidation in a JSR. Overall, agreement between the predictions and measurements is obtained, with a maximum deviation of 30%. In this present work, the integrated reduction scheme is demonstrated to be applicable to small-scale mechanism reduction while maintaining the corresponding accuracy for a given application. The compact model proposed here is ready to be used in ethylene flame simulations.

Keywords: Chemical kinetics, Mechanism reduction, Ethylene, Small-scale mechanism.

Nomenclatures

| | |
|-------|---------------------------|
| h | Height above burner |
| P | Pressure |
| PSR | Perfectly-Stirred Reactor |
| T | Temperature |
| t_R | Residence time |

Abbreviations

| | |
|-------|--|
| 0-D | Zero Dimensional |
| 1-D | One-Dimensional |
| CFD | Computational Fluid Dynamics |
| DRG | Directed Relation Graph |
| DRGEP | Direct Relation Graph with Error Propagation |
| ID | Ignition Delay |
| JSR | Jet-Stirred Reactor |

1. Introduction

To date, the oxidation and pyrolysis of ethylene have been widely studied using both experimental and kinetic modelling approaches [1-6]. Ethylene is a main intermediate in the combustion of aliphatic hydrocarbons and aromatic compounds [1, 3, 6, 7]. It plays an important role in polycyclic aromatic hydrocarbons and soot formation processes [8]. In addition, ethylene is also produced from the combustion of larger hydrocarbons through β -scission process [6, 7]. In view of the importance of ethylene chemistry in the combustion of large hydrocarbons and various practical fuels, a kinetically accurate ethylene model is expected to be useful in aiding fuel combustion and soot formation predictions for multi-dimensional computational fluid dynamics (CFD) modelling studies.

In a previous work, an integrated chemical kinetic mechanism reduction scheme was developed to generate reduced models for large mechanisms such as the diesel and biodiesel fuel surrogate models [9-11]. Based on its promising performance on large-scale mechanism reduction, the aim of this study is to examine the applicability of the scheme on reduction of small-scale mechanism using a 111-species detailed ethylene model developed by Wang et al. [12]. It is noted that application of a detailed model in multi-dimensional CFD simulations involves massive amounts of computational memory. Thus, a sufficiently compact kinetic model is pertinent to capture the combustion phenomena with fair confidence. Here, the newly developed reduced model is then applied in one-dimensional (1-D) simulations to simulate ethylene/air flame in a pre-mixed flat flame burner at varied equivalence ratio (Φ). The fidelity of the reduced model is also further evaluated in zero-dimensional (0-D) simulations with respect to ignition delay (ID) and species concentration predictions.

2. Development of Reduced Ethylene Model

The detailed ethylene mechanism [12] which consists of 111 species with 784 elementary reactions is selected as the base model. Here, the capability of the mechanism in flame temperature predictions is designated as the basis for mechanism reduction using an integrated reduction scheme illustrated in Fig. 1.

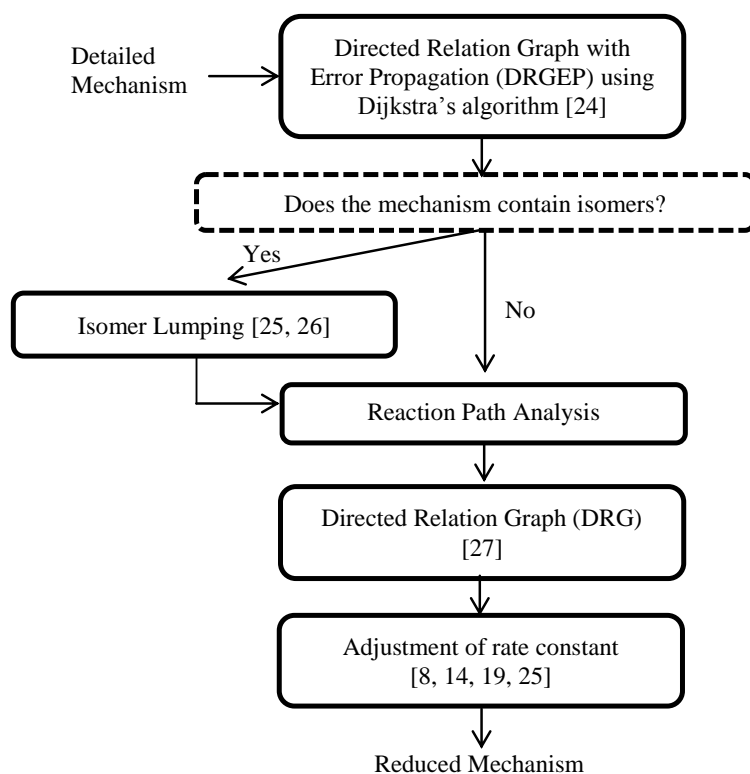


Fig. 1. Integrated chemical kinetic mechanism reduction scheme.

The operating conditions used in the reduction procedure are illustrated in Table 1. Further descriptions of the reduction scheme are detailed in the previous work [9-11].

Table 1. Operating conditions applied in mechanism reduction and model validations in 1-D simulations.

| Parameters | Range considered |
|------------|----------------------------|
| Φ (-) | 0.5 - 2.5 (0.1 increments) |
| P (atm) | 1 |
| T (K) | 300 |
| h (mm) | 8.5 |

P , T , h denote initial pressure, initial temperature and height above burner, respectively.

DRGEP is first applied in the reduction procedure to filter a subset of undesirable species from the mechanism by using a universally specifiable threshold value. As discussed in the previous reduction work, CO, CO₂, HCO, HO₂, H₂ and N₂ are designated as the 'target species' to determine their shortest pathways to all other species [9-11]. Consequently, a resulting mechanism with 55 species is generated, and the maximum deviation in flame temperature predictions is maintained to within 2.5% as compared to the computations of the detailed model.

Following that, reaction pathway analysis is performed and the major reaction pathways during ethylene combustion are illustrated in Fig. 2. Isomer lumping is neglected here as there are no isomers present in the mechanism.

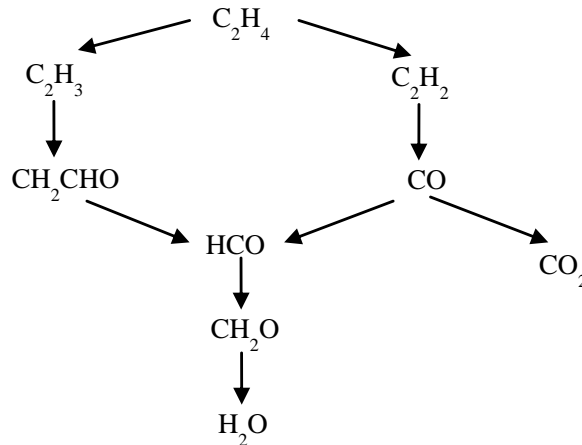


Fig. 2. Main reaction pathways during ethylene (C_2H_4) combustion.

Upon elimination of species which have lost pathway connections from the major species through DRG, adjustment of reaction rate constant is performed so that the influence of the eliminated reactions is integrated in the Arrhenius rate constants of the retained reactions to maintain model accuracy [8, 13, 14]. Here, A-factor constant for reaction ' $C_2H_2 + O = CH_2 + CO$ ' is optimised to improve the flame temperature predictions throughout the tested Φ range.

As a result, a reduced ethylene model comprising 27 species with 147 elementary reactions is produced, as illustrated in Table A.1 in Appendix. The application of the reduction scheme has successfully reduced the size of the detailed model by 75.7% and 81.3% in terms of the total number of species and elementary reactions, respectively. Successively, the reduced model is carried forward to the next section for model validations in 1-D simulations.

3. Model validation in 1-D laminar flame-speed simulations

In this section, the flame temperatures of ethylene combustion under a wide range of Φ are investigated. The simulation setup is selected based on the experimental work of Ivarsson [15]. The operating conditions applied here are illustrated in Table 1.

The premixed laminar burner stabilised flame model of CHEMKIN-PRO software is employed. It is commonly used to model chemical kinetics and transport processes in flames and is useful in computing temperature as well as species profiles under laminar premixed flame configurations. In this work, the laminar flame is modelled in one dimension as the temperature distribution, velocity and chemical composition within the flame is almost consistent perpendicular to the direction of flow [15]. This approach is also commonly used in other flame modelling studies [16-18].

The flame temperature profiles computed by the reduced ethylene model are compared with those of the detailed model in Fig. 3. Good agreement between

the reduced and detailed models is observed with a maximum deviation of 2.8% in flame temperature predictions. This variation is partly due to the elimination of some intermediate species during the mechanism reduction procedure. These species were found to have very low concentrations and net production rates during the key combustion event. However, the deviation becomes more significant at higher Φ owing to the increased reactivity level of these eliminated species. Despite the slight deviation, the results obtained here have demonstrated an acceptable compromise in terms of mechanism size and results accuracy over the parameter range of interest. Apart from these, a 97% reduction in computational time is obtained for each simulation as compared to that of the detailed model.

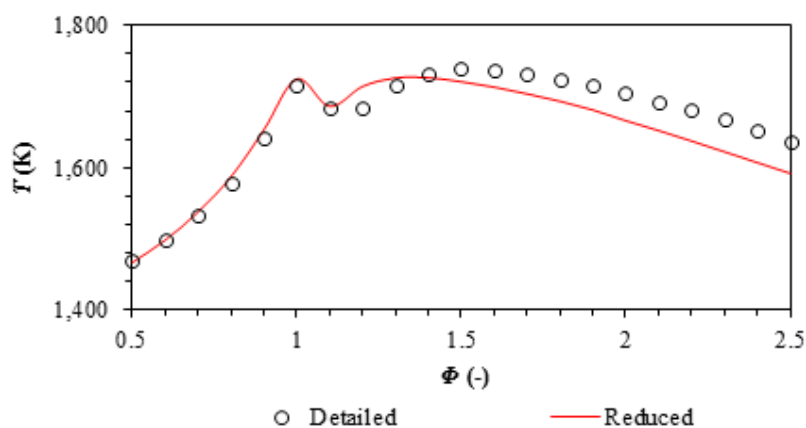


Fig. 3. Comparison of the flame temperature profiles generated by the reduced and detailed ethylene mechanisms.

4. Further validations in 0-D chemical kinetic simulations

Subsequently, the 27-species reduced ethylene model developed in the previous section is further validated with respect to IDs (Fig. 4), species mole fractions under auto-ignition (Fig. 5) and jet-stirred reactor (JSR) (Fig. 6) conditions as well as species mole fractions against JSR experimental data of Dagaut et al. [3] (Fig. 7). The operating conditions applied in these 0-D simulations are depicted in Table 2 which cover low to high pressures and temperatures so that the model can be used in wider range of CFD applications.

Here, closed homogeneous batch reactor and perfectly-stirred reactor (PSR) models of CHEMKIN-PRO software are employed. Closed homogeneous batch reactor model is used to simulate dynamic reactor conditions in which the controlling conditions vary with respect to time. Here, IDs predicted by the kinetic model in a constant volume system along with the key species profiles are calculated as a function of time under auto-ignition condition. In contrast, the open PSR model, which is also known as a continuously stirred tank reactor, is applied to simulate steady-state reactor systems from which species profiles as a function of ambient temperature are computed in this work. Hence, this model is employed here to model steady-state extinction of the combustion process under JSR condition [19].

Table 2. Operating conditions applied in 0-D simulations.

| Conditions | Parameters | Range Considered |
|----------------------------|------------|-------------------------------|
| Auto-ignition ^a | Φ (-) | 0.5, 1.0, 2.0 |
| | P (bar) | 13.5, 41.0 |
| | T (K) | 650 - 1350 (100 K increments) |
| JSR ^a | Φ (-) | 0.5, 1.0, 2.0 |
| | P (bar) | 13.5, 41.0 |
| | t_R (s) | 1 |
| JSR ^b | Φ (-) | 2 |
| | P (atm) | 5 |
| | T (K) | 1080 |

t_R denotes residence time; ^aOperating conditions selected for model validations against the computations of the detailed model; ^bOperating conditions selected for model validations according to the experimental results of fuel oxidation in a JSR.

4.1. Validations against detailed model under auto-ignition and JSR conditions

Comparisons of ID computed by the reduced and detailed models are demonstrated in Fig. 4. Good agreements between the models are observed throughout the test conditions, with a maximum deviation recorded at 10%. This is reasonable considering that the present reduced model has not been developed using the auto-ignition and JSR conditions as the basis for mechanism reduction.

Furthermore, satisfactory results are also obtained in species concentration predictions between the reduced and detailed models for fuel oxidations under auto-ignition and JSR conditions, with maximum deviations retained to within 20%. The results are demonstrated in Figs. 5 and 6, respectively. Here, only results for initial pressure of 41 bar and Φ of 1 are presented since similar temporal evolution trends are obtained for other conditions.

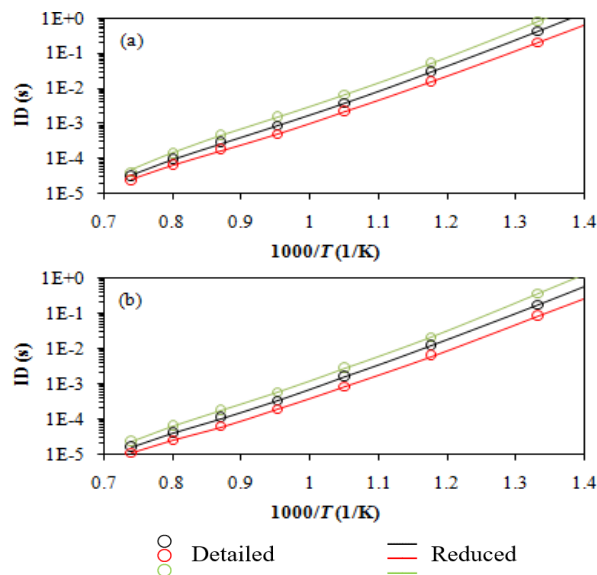


Fig. 4. Comparisons of IDs predicted by the reduced and detailed ethylene mechanisms for initial P of (a) 13.5 bar and (b) 41 bar, with Φ of 0.5 (green), 1.0 (black) and 2 (red).

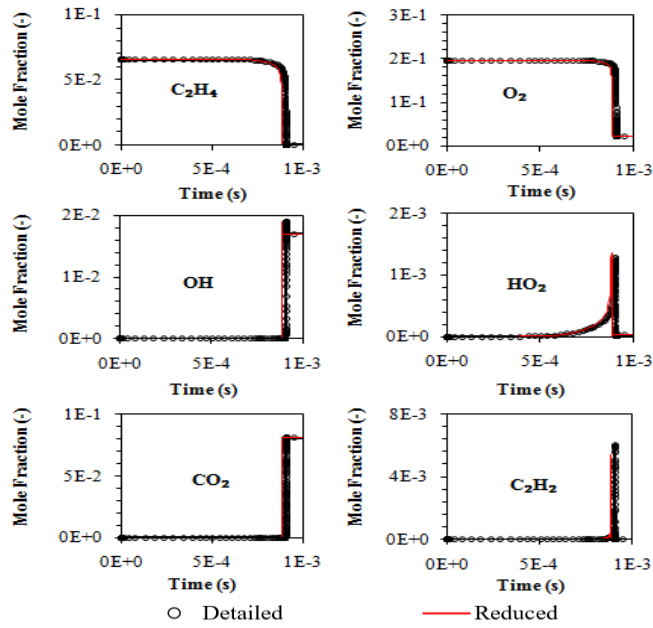


Fig. 5. Comparison of species profiles of the reduced and detailed ethylene mechanisms under auto-ignition condition as a function of time, with initial P of 41 bar, initial T of 1050 K and Φ of 1.

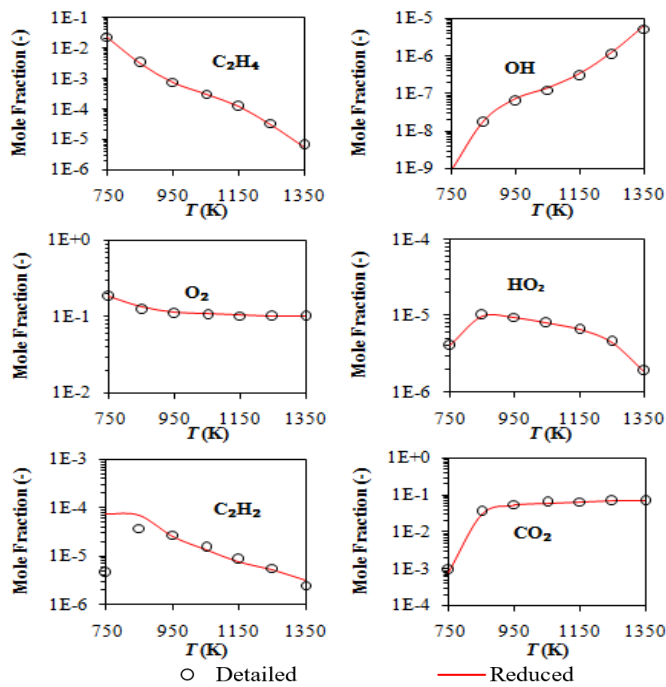


Fig. 6. Comparison of species profiles of the reduced and detailed ethylene mechanisms under JSR condition as a function of T , with initial P of 41 bar and Φ of 1.

4.2. Validations against JSR experimental measurements

In addition, the reduced ethylene model is further validated using the JSR experimental results of Dagaut et al. [3]. The experimental operating conditions are illustrated in Table 2. The initial fuel mixtures consist of 0.15% ethylene, 0.225% oxygen and 99.625% nitrogen by volume. The validation results are depicted in Fig. 7 by comparing the species concentration predictions to the experimental data for fuel-oxygen mixtures, diluted by nitrogen. Species such as CH_4 , CO_2 , C_2H_2 , C_2H_4 , C_2H_6 and H_2 are validated to ensure that the reduced model is able to provide a reasonable representation of the kinetics of the fuel oxidation.

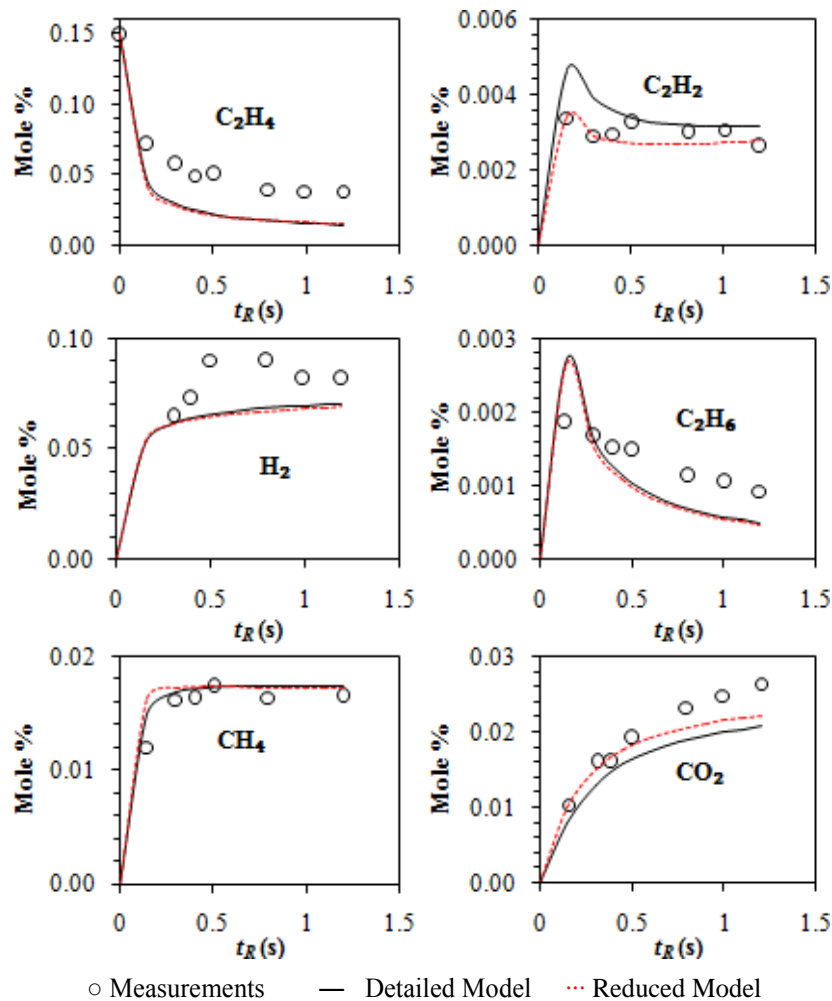


Fig. 7. Computed and experimental species mole fraction obtained from the oxidation of 0.15 % C_2H_4 in a JSR at P of 5 atm and Φ of 2.

The results in Fig. 7 show that the reduced model is able to reproduce the species profiles and kinetics of the fuel oxidation satisfactorily. The maximum deviation between the predictions and measurements is approximately 30 %. The discrepancies could potentially be attributed to the uncertainties in the

experiments as well as the kinetics of the detailed model itself. For instance, it has been reported that some of the reaction rate coefficients of the kinetic model have uncertainty factors from a range of 1.2 to 4 [20]. These kinetic uncertainties may be readily propagated when the model is applied to a wide range of combustion conditions. The computed deviation range is considered to be acceptable as variations of species concentrations can also reach as high as one order of magnitude of the absolute value [21-23]. In Fig. 7, a decreasing trend in fuel (C_2H_4) concentration predictions is obtained when the mean t_R increases. However, it is also observed that C_2H_4 concentrations are under-predicted when mean t_R is greater than 0.15 s. As a result of the different fuel consumption rate, the formations of CO_2 and H_2 also vary from the experimental profiles. Apart from the comparison with the experimental data, the species profile trends computed by the reduced model are found to be consistent with those predicted by the detailed model. There is no substantial loss in chemical fidelity through the mechanism reduction procedure. Despite the variation between the computations and measurements, the computational results of the reduced model are deemed acceptable in view of its simplified fuel chemistries.

5. Conclusions

An investigation on the applicability of the integrated chemical kinetic mechanism reduction scheme on small-scale mechanism has been performed. Here, a detailed ethylene model with 111 species is applied as the base model for mechanism reduction. A reduced ethylene model with 27 species and 147 elementary reactions is successfully generated while reductions of 75.7 % and 81.3 % in terms of total number of species and elementary reactions, respectively, are achieved in comparison to the detailed model. Successively, flame temperatures under a wide range of Φ are examined in 1-D laminar flame-speed simulations. Close agreements are achieved between the reduced and detailed models, with a maximum deviation of 2.8% in flame temperature predictions. Accordingly, further validations of the reduced model in 0-D simulations are performed. Satisfactory results in ID as well as species profile predictions are obtained under both auto-ignition and JSR conditions. The maximum deviation between the predictions of the reduced and detailed models is maintained to within 20% throughout the test conditions. Apart from that, fidelity of the reduced model is also assessed using the experimental data of ethylene oxidation in a JSR. The experimental species concentration profiles are reasonably reproduced while maximum relative error of 30% is recorded between the computations and measurements. The integrated reduction scheme is shown to be appropriate for small-scale mechanism reduction with reasonable accuracy. The reduced ethylene model proposed in this work can be applied in numerical simulations to study ethylene flame.

Acknowledgements

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Appendix
Table A.1. The reduced ethylene mechanism.
Units are in mole, cm, s, K and cal.

| Reaction | Reaction Considered | A | b | E |
|----------|---------------------|----------|-------|----------|
| 1 | H+O2=O+OH | 2.64E+16 | -0.7 | 17041 |
| 2 | O+H2=H+OH | 4.59E+04 | 2.7 | 6260 |
| 3 | OH+H2=H+H2O | 1.73E+08 | 1.5 | 3430 |
| 4 | OH+OH=O+H2O | 3.97E+04 | 2.4 | -2110 |
| 5 | H+H+M=H2+M | 1.78E+18 | -1 | 0 |
| | H2 | Enhanced | by | 0.00E+00 |
| | H2O | Enhanced | by | 0.00E+00 |
| | CO2 | Enhanced | by | 0.00E+00 |
| 6 | H+H+H2=H2+H2 | 9.00E+16 | -0.6 | 0 |
| 7 | H+H+H2O=H2+H2O | 5.62E+19 | -1.2 | 0 |
| 8 | H+H+CO2=H2+CO2 | 5.50E+20 | -2 | 0 |
| 9 | H+OH+M=H2O+M | 4.40E+22 | -2 | 0 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.30E+00 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO2 | Enhanced | by | 3.60E+00 |
| 10 | O+H+M=OH+M | 9.43E+18 | -1 | 0 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 1.20E+01 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO2 | Enhanced | by | 3.60E+00 |
| 11 | O+O+M=O2+M | 1.20E+17 | -1 | 0 |
| | H2 | Enhanced | by | 2.40E+00 |
| | H2O | Enhanced | by | 1.54E+01 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO2 | Enhanced | by | 3.60E+00 |
| 12 | H+O2(+M)=HO2(+M) | 5.12E+12 | 0.4 | 0 |
| | O2 | Enhanced | by | 8.50E-01 |
| | H2O | Enhanced | by | 1.19E+01 |
| | CO | Enhanced | by | 1.09E+00 |
| | CO2 | Enhanced | by | 2.18E+00 |
| 13 | H2+O2=HO2+H | 5.92E+05 | 2.4 | 53502 |
| 14 | OH+OH(+M)=H2O2(+M) | 1.11E+14 | -0.4 | 0 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO2 | Enhanced | by | 3.60E+00 |
| 15 | HO2+H=O+H2O | 3.97E+12 | 0 | 671 |
| 16 | HO2+H=OH+OH | 7.48E+13 | 0 | 295 |
| 17 | HO2+O=OH+O2 | 4.00E+13 | 0 | 0 |
| 18 | HO2+HO2=O2+H2O2 | 1.30E+11 | 0 | -1630 |
| 19 | HO2+HO2=O2+H2O2 | 3.66E+14 | 0 | 12000 |
| 20 | OH+HO2=H2O+O2 | 1.41E+18 | -1.8 | 60 |
| 21 | OH+HO2=H2O+O2 | 1.12E+85 | -22.3 | 26900 |
| 22 | OH+HO2=H2O+O2 | 5.37E+70 | -16.7 | 32900 |
| 23 | OH+HO2=H2O+O2 | 2.51E+12 | 2 | 40000 |
| 24 | OH+HO2=H2O+O2 | 1.00+136 | -40 | 34800 |
| 25 | H2O2+H=HO2+H2 | 6.05E+06 | 2 | 5200 |
| 26 | H2O2+H=OH+H2O | 2.41E+13 | 0 | 3970 |
| 27 | H2O2+O=OH+HO2 | 9.63E+06 | 2 | 3970 |
| 28 | H2O2+OH=HO2+H2O | 2.00E+12 | 0 | 427 |
| 29 | H2O2+OH=HO2+H2O | 2.67E+41 | -7 | 37600 |
| 30 | CO+O(+M)=CO2(+M) | 1.36E+10 | 0 | 2384 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 1.20E+01 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO2 | Enhanced | by | 3.60E+00 |
| 31 | CO+OH=CO2+H | 7.05E+04 | 2.1 | -355.7 |

| | | | | |
|----|---|----------|------|----------|
| 32 | CO+OH=CO ₂ +H | 5.76E+12 | -0.7 | 331.8 |
| 33 | CO+O ₂ =CO ₂ +O | 1.12E+12 | 0 | 47700 |
| 34 | CO+HO ₂ =CO ₂ +OH | 1.57E+05 | 2.2 | 17942.6 |
| 35 | HCO+H=CO+H ₂ | 1.20E+14 | 0 | 0 |
| 36 | HCO+O=CO+OH | 3.00E+13 | 0 | 0 |
| 37 | HCO+O=CO ₂ +H | 3.00E+13 | 0 | 0 |
| 38 | HCO+OH=CO+H ₂ O | 3.02E+13 | 0 | 0 |
| 39 | HCO+M=CO+H+M | 1.87E+17 | -1 | 17000 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 0.00E+00 |
| | CO | Enhanced | by | 1.75E+00 |
| | CO ₂ | Enhanced | by | 3.60E+00 |
| 40 | HCO+H ₂ O=CO+H+H ₂ O | 2.24E+18 | -1 | 17000 |
| 41 | HCO+O ₂ =CO+HO ₂ | 1.20E+10 | 0.8 | -727 |
| 42 | CO+H ₂ (+M)=CH ₂ O(+M) | 4.30E+07 | 1.5 | 79600 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 6.00E+00 |
| | CH ₄ | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO ₂ | Enhanced | by | 2.00E+00 |
| | C ₂ H ₆ | Enhanced | by | 3.00E+00 |
| 43 | HCO+H(+M)=CH ₂ O(+M) | 1.09E+12 | 0.5 | -260 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 6.00E+00 |
| | CH ₄ | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO ₂ | Enhanced | by | 2.00E+00 |
| | C ₂ H ₆ | Enhanced | by | 3.00E+00 |
| 44 | CH ₂ +H(+M)=CH ₃ (+M) | 2.50E+16 | -0.8 | 0 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 6.00E+00 |
| | CH ₄ | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO ₂ | Enhanced | by | 2.00E+00 |
| | C ₂ H ₆ | Enhanced | by | 3.00E+00 |
| 45 | CH ₂ +O=HCO+H | 8.00E+13 | 0 | 0 |
| 46 | CH ₂ +OH=CH ₂ O+H | 2.00E+13 | 0 | 0 |
| 47 | CH ₂ +H ₂ =H+CH ₃ | 5.00E+05 | 2 | 7230 |
| 48 | CH ₂ +O ₂ =HCO+OH | 1.06E+13 | 0 | 1500 |
| 49 | CH ₂ +O ₂ =CO ₂ +H+H | 2.64E+12 | 0 | 1500 |
| 50 | CH ₂ +HO ₂ =CH ₂ O+OH | 2.00E+13 | 0 | 0 |
| 51 | CH ₂ +CO(+M)=CH ₂ CO(+M) | 8.10E+11 | 0.5 | 4510 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 6.00E+00 |
| | CH ₄ | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO ₂ | Enhanced | by | 2.00E+00 |
| | C ₂ H ₆ | Enhanced | by | 3.00E+00 |
| 52 | CH ₂ +CH ₂ =C ₂ H ₂ +H ₂ | 3.20E+13 | 0 | 0 |
| 53 | CH ₂ O+H(+M)=CH ₃ O(+M) | 5.40E+11 | 0.5 | 2600 |
| | H ₂ | Enhanced | by | 2.00E+00 |
| | H ₂ O | Enhanced | by | 6.00E+00 |
| | CH ₄ | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO ₂ | Enhanced | by | 2.00E+00 |
| | C ₂ H ₆ | Enhanced | by | 3.00E+00 |
| 54 | CH ₂ O+H=HCO+H ₂ | 2.30E+10 | 1.1 | 3275 |
| 55 | CH ₂ O+O=HCO+OH | 3.90E+13 | 0 | 3540 |
| 56 | CH ₂ O+OH=HCO+H ₂ O | 3.43E+09 | 1.2 | -447 |
| 57 | CH ₂ O+O ₂ =HCO+HO ₂ | 1.00E+14 | 0 | 40000 |
| 58 | CH ₂ O+HO ₂ =HCO+H ₂ O ₂ | 1.00E+12 | 0 | 8000 |
| 59 | CH ₃ +H(+M)=CH ₄ (+M) | 1.27E+16 | -0.6 | 383 |
| | H ₂ | Enhanced | by | 2.00E+00 |

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|----|------------------------|----------|------|----------|
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| 60 | CH3+O=CH2O+H | 8.43E+13 | 0 | 0 |
| 61 | CH3+OH=CH2+H2O | 5.60E+07 | 1.6 | 5420 |
| 62 | CH3+O2=O+CH3O | 3.08E+13 | 0 | 28800 |
| 63 | CH3+O2=OH+CH2O | 3.60E+10 | 0 | 8940 |
| 64 | CH3+HO2=CH4+O2 | 1.00E+12 | 0 | 0 |
| 65 | CH3+HO2=CH3O+OH | 1.34E+13 | 0 | 0 |
| 66 | CH3+H2O2=CH4+HO2 | 2.45E+04 | 2.5 | 5180 |
| 67 | CH3+HCO=CH4+CO | 8.48E+12 | 0 | 0 |
| 68 | CH3+CH2O=CH4+HCO | 3.32E+03 | 2.8 | 5860 |
| 69 | CH3+CH2=C2H4+H | 4.00E+13 | 0 | 0 |
| 70 | CH3+CH3(+M)=C2H6(+M) | 2.12E+16 | -1 | 620 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| 71 | CH3+CH3=H+C2H5 | 4.99E+12 | 0.1 | 10600 |
| 72 | CH3O+H=CH2O+H2 | 2.00E+13 | 0 | 0 |
| 73 | CH3O+H=CH3+OH | 3.20E+13 | 0 | 0 |
| 74 | CH3O+O=CH2O+OH | 1.00E+13 | 0 | 0 |
| 75 | CH3O+OH=CH2O+H2O | 5.00E+12 | 0 | 0 |
| 76 | CH3O+O2=CH2O+HO2 | 4.28E-13 | 7.6 | -3530 |
| 77 | CH4+H=CH3+H2 | 6.60E+08 | 1.6 | 10840 |
| 78 | CH4+O=CH3+OH | 1.02E+09 | 1.5 | 8600 |
| 79 | CH4+OH=CH3+H2O | 1.00E+08 | 1.6 | 3120 |
| 80 | CH4+CH2=CH3+CH3 | 2.46E+06 | 2 | 8270 |
| 81 | C2H3(+M)=C2H2+H(+M) | 3.86E+08 | 1.6 | 37048.2 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| | C2H2 | Enhanced | by | 3.00E+00 |
| | C2H4 | Enhanced | by | 3.00E+00 |
| 82 | C2H2+O=CH2+CO | 4.08E+07 | 2 | 1900 |
| 83 | C2H2+OH=CH2CO+H | 2.18E-04 | 4.5 | -1000 |
| 84 | C2H2+OH=CH3+CO | 4.83E-04 | 4 | -2000 |
| 85 | C2H2+HCO=C2H3+CO | 1.00E+07 | 2 | 6000 |
| 86 | CH2CO+H(+M)=CH2CHO(+M) | 3.30E+14 | -0.1 | 8500 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| | C2H2 | Enhanced | by | 3.00E+00 |
| | C2H4 | Enhanced | by | 3.00E+00 |
| 87 | CH2CO+H=CH3+CO | 1.50E+09 | 1.4 | 2690 |
| 88 | CH2CO+O=CH2+CO2 | 1.75E+12 | 0 | 1350 |
| 89 | C2H3+H(+M)=C2H4(+M) | 6.08E+12 | 0.3 | 280 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |

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|-----|-----------------------|----------|------|----------|
| | C2H2 | Enhanced | by | 3.00E+00 |
| | C2H4 | Enhanced | by | 3.00E+00 |
| 90 | C2H3+H=C2H2+H2 | 9.00E+13 | 0 | 0 |
| 91 | C2H3+O=CH2CO+H | 4.80E+13 | 0 | 0 |
| 92 | C2H3+O=CH3+CO | 4.80E+13 | 0 | 0 |
| 93 | C2H3+OH=C2H2+H2O | 3.01E+13 | 0 | 0 |
| 94 | C2H3+O2=C2H2+HO2 | 1.34E+06 | 1.6 | -383.4 |
| 95 | C2H3+O2=CH2CHO+O | 3.00E+11 | 0.3 | 11 |
| 96 | C2H3+O2=HCO+CH2O | 4.60E+16 | -1.4 | 1010 |
| 97 | C2H3+HO2=CH2CHO+OH | 1.00E+13 | 0 | 0 |
| 98 | C2H3+H2O2=C2H4+HO2 | 1.21E+10 | 0 | -596 |
| 99 | C2H3+HCO=C2H4+CO | 9.03E+13 | 0 | 0 |
| 100 | C2H3+CH3=C2H2+CH4 | 3.92E+11 | 0 | 0 |
| 101 | C2H3+CH3(+M)=C3H6(+M) | 2.50E+13 | 0 | 0 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| | C2H2 | Enhanced | by | 3.00E+00 |
| | C2H4 | Enhanced | by | 3.00E+00 |
| 102 | C2H3+C2H3=C2H2+C2H4 | 9.60E+11 | 0 | 0 |
| 103 | CH2CHO=CH3+CO | 7.80E+41 | -9.1 | 46900 |
| 104 | CH2CHO+H=CH3+HCO | 9.00E+13 | 0 | 0 |
| 105 | CH2CHO+H=CH2CO+H2 | 2.00E+13 | 0 | 4000 |
| 106 | CH2CHO+O=CH2CO+OH | 2.00E+13 | 0 | 4000 |
| 107 | CH2CHO+OH=CH2CO+H2O | 1.00E+13 | 0 | 2000 |
| 108 | CH2CHO+O2=CH2CO+HO2 | 1.40E+11 | 0 | 0 |
| 109 | CH2CHO+O2=CH2O+CO+OH | 1.80E+10 | 0 | 0 |
| 110 | CH2OCH2=CH3+HCO | 3.63E+13 | 0 | 57200 |
| 111 | CH2OCH2=CH4+CO | 1.21E+13 | 0 | 57200 |
| 112 | CH2OCH2+H=C2H3+H2O | 5.00E+09 | 0 | 5000 |
| 113 | CH2OCH2+H=C2H4+OH | 9.51E+10 | 0 | 5000 |
| 114 | C2H4+H(+M)=C2H5(+M) | 1.37E+09 | 1.5 | 1355 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| 115 | C2H4+H=C2H3+H2 | 5.07E+07 | 1.9 | 12950 |
| 116 | C2H4+O=C2H3+OH | 1.51E+07 | 1.9 | 3740 |
| 117 | C2H4+O=CH3+HCO | 1.92E+07 | 1.8 | 220 |
| 118 | C2H4+O=CH2+CH2O | 3.84E+05 | 1.8 | 220 |
| 119 | C2H4+OH=C2H3+H2O | 3.60E+06 | 2 | 2500 |
| 120 | C2H4+HCO=C2H5+CO | 1.00E+07 | 2 | 8000 |
| 121 | C2H4+CH3=C2H3+CH4 | 2.27E+05 | 2 | 9200 |
| 122 | C2H4+CH3=nC3H7 | 3.30E+11 | 0 | 7700 |
| 123 | C2H4+O2=C2H3+HO2 | 4.22E+13 | 0 | 60800 |
| 124 | C2H4+HO2=CH2OCH2+OH | 2.82E+12 | 0 | 17100 |
| 125 | C2H5+H(+M)=C2H6(+M) | 5.21E+17 | -1 | 1580 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| 126 | C2H5+H=C2H4+H2 | 2.00E+12 | 0 | 0 |
| 127 | C2H5+O=CH3+CH2O | 1.60E+13 | 0 | 0 |
| 128 | C2H5+O2=C2H4+HO2 | 2.00E+10 | 0 | 0 |
| 129 | C2H5+HO2=C2H6+O2 | 3.00E+11 | 0 | 0 |
| 130 | C2H5+HO2=C2H4+H2O2 | 3.00E+11 | 0 | 0 |

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| 131 | $C_2H_5+HO_2=CH_3+CH_2O+OH$ | 2.40E+13 | 0 | 0 |
| 132 | $C_2H_5+H_2O_2=C_2H_6+HO_2$ | 8.70E+09 | 0 | 974 |
| 133 | $C_2H_6+H=C_2H_5+H_2$ | 1.15E+08 | 1.9 | 7530 |
| 134 | $C_2H_6+O=C_2H_5+OH$ | 8.98E+07 | 1.9 | 5690 |
| 135 | $C_2H_6+OH=C_2H_5+H_2O$ | 3.54E+06 | 2.1 | 870 |
| 136 | $C_2H_6+CH_3=C_2H_5+CH_4$ | 6.14E+06 | 1.7 | 10450 |
| 137 | $C_3H_6+H(+M)=nC_3H_7(+M)$ | 1.33E+13 | 0 | 3260.7 |
| | H2 | Enhanced | by | 2.00E+00 |
| | H2O | Enhanced | by | 6.00E+00 |
| | CH4 | Enhanced | by | 2.00E+00 |
| | CO | Enhanced | by | 1.50E+00 |
| | CO2 | Enhanced | by | 2.00E+00 |
| | C2H6 | Enhanced | by | 3.00E+00 |
| 138 | $C_3H_6+H=C_2H_4+CH_3$ | 8.00E+21 | -2.4 | 11180 |
| 139 | $C_3H_6+O=C_2H_4CO+CH_3+H$ | 8.00E+07 | 1.6 | 327 |
| 140 | $C_3H_6+O=C_2H_5+HCO$ | 3.50E+07 | 1.6 | -972 |
| 141 | $nC_3H_7+H=C_2H_5+CH_3$ | 3.70E+24 | -2.9 | 12505 |
| 142 | $nC_3H_7+H=C_3H_6+H_2$ | 1.80E+12 | 0 | 0 |
| 143 | $nC_3H_7+O=C_2H_5+CH_2O$ | 9.60E+13 | 0 | 0 |
| 144 | $nC_3H_7+OH=C_3H_6+H_2O$ | 2.40E+13 | 0 | 0 |
| 145 | $nC_3H_7+O_2=C_3H_6+HO_2$ | 9.00E+10 | 0 | 0 |
| 146 | $nC_3H_7+HO_2=C_2H_5+OH+CH_2O$ | 2.40E+13 | 0 | 0 |
| 147 | $nC_3H_7+CH_3=CH_4+C_3H_6$ | 1.10E+13 | 0 | 0 |