O₂/CH₄ Kinetic Mechanisms for Aerospace Applications at Low Pressure and Temperature, Validity Ranges and Comparison

Angelo Minotti
“Sapienza” University of Rome, Italy

1. Introduction

In recent years, the propellant combination O₂/CH₄ has received attraction in Japan, USA and Europe as a propellant combination for attitude control, upper stage, booster engines and microcombustion systems. Moreover, this propellant pair is of interest for exploration missions (Stone et al., 2008; Hulbert et al., 2008; Arione, 2010; Kawashima et al., 2009) and for in-space propulsion systems. The reason of the exploration/in-space interest stays in the fact that all the missions with a reduced requirement of thermal management and propellant losses through evaporation will surely profit from a O₂/CH₄ based propulsion system. Microcombustion, for space and terrestrial use, takes profit from the O₂/CH₄ propellant combination thanks to its availability, easy to handle, and knowledge. Besides the interest in methane for space-terrestrial applications, this propellant being a renewable bio-fuel has seen rising interest for both economic and ecologic reasons.

Microthrusters were associated with the emergence of micro- and nano-satellite concepts, in which satellites are conceived capable of the same or similar performance of conventional satellites within a much smaller package/weight by using MEMS technology (Micro Electrical Mechanical System). This increasing interest in MEMS devices, in particular those based or including combustion/chemical propulsion, is also forcing new needs and problems to emerge (Janson, 1994; DeGroot & Oleson, 1996; Mueller, 1997; Bruno, 2001). One of these is the heat loss through combustor walls due to the much increased surface/volume ratio reducing the actual energy available for the cycle chosen: this explains the sometimes startlingly low temperatures observed experimentally (Minotti et al., 2009; Bruno, 2001; Cozzi, 2007; Cozzi & Caratti, 2007; Bruno et al., 2003; Cozzi et al., 2007). Even when equivalence ratios (Φ) are close to one, these call for kinetics capable of realistically predicting ignition delays times and combustion efficiency at a reasonable computational cost.

The requirement to predict with sufficient accuracy combustion performance and heat load to the chamber walls has lead, in the last decade, the numerical modelling to rapidly become an essential part of combustion research and development programs, and there has been an accelerating evolution from the use of single-step empirical kinetics, to the use of lumped semiglobal (multistep) models (Wesbrook & Dryer, 1981; Bowman, 1986), and finally to the inclusion of full detailed chemical kinetic mechanisms to better simulate chemistry interactions. In addition, detailed mechanisms have been developed and validated for the
simplest fuel molecules (Westbrook and Dryer, 1981) and are not available for most practical fuels. Finally there are many occasions where the great amount of chemical information produced by a detailed reaction mechanism is not necessary and a simple mechanism will suffice together with the fact that 3D combustors cannot easily include detailed kinetic mechanisms because the computational costs of such a treatment would be much too great.

Several works concerning hydrocarbon kinetics are present in literature (Paczko et al., 1988; Westbrook Dryer, 1981; Kee et al., 1985; Heffington, 1997; Hautman, 1981; Trevino & Mendez, 1992; Dagaut, 1991), and the work of Gardiner (1999) is important to understand the hydrocarbon oxidation chemistry, in particular for what concerns differences between methane and other hydrocarbons. The state of the art for methane reactions is by the Gas Research Institute, periodically releasing new updated versions of its detailed methane-air reaction mechanism (GRI-Mech, http://www.me.berkeley.edu/gri_mech/ or http://www.gri.org).

Said that, this work indicates two ways to “define/build” a reaction mechanism and presents five reaction mechanisms adopted in hydrocarbons simulations: one global, two 2-steps, one multisteps and one detailed reaction mechanism.

All of them are compared with the detailed GRI-Mech3.0 reaction mechanism (GRI-Mech, 1999) by means of the CHEMKin3.7 tool (the Aurora application) to figure out the ignition delay time and final temperature differences, in order to understand the problems, and limits, related to a delicate topic as the reaction mechanism modelling is.

Section 2 provides few important hints to define a reaction mechanism, section 3 shows the five reaction mechanisms which are studied, while section 4 and 5 report comparisons and their validity ranges.

2. Reaction mechanism definition

A reaction mechanism may be obtained following, in general, two different paths, depending on whether a reduced mechanism or a semiglobal mechanism is required.

If a reduced mechanism is the goal, the “recipe” might be summarized by:

1. definition of the starting detailed mechanism;
2. definition of the operating conditions;
3. sensitivity analysis to reduce the reactions number.

(The sensitivity \( Y_{X_i} \) analysis is the study of how the variation (uncertainty) in the output (Y) of a mathematical model can be apportioned, qualitatively or quantitatively, to different sources (X_i) of variation in the input of a model, that is \( Y_{X_i} = \frac{\partial Y}{\partial X_i} \); this measure tells how sensitive the output is to a perturbation of the input. If a measure independent from the units used for Y and X_i is needed, \( S_{X_i} = \left( \frac{X_i}{Y} \right) \left( \frac{\partial Y}{\partial X_i} \right) \) can be used, where \( \bar{X}_i \) is the nominal (or central, if a range is known) value of factor X_i and \( \bar{Y} \) is the value taken by Y when all input factors are at their nominal value. In the reaction mechanisms the sensitivity analysis is carried out analysing the sensitivity of some species or of some reaction velocities on the overall mechanism).

On the other hand, if a semiglobal mechanism is the goal, the “recipe” might be summarized in the following way:

1. definition of species of interest (they affect the reaction enthalpy and then the final temperature);
2. Definition of reactions (and their number);
3. Definition of operating conditions;
4. Modification of Arrhenius variables ($A$, $n$ and $E_a$) to obtain the required ignition delay.

Any simplified reaction mechanism must be capable of reproducing experimental flame properties over the range of operating conditions under consideration. Hence, in both the paths the operating conditions definition plays a fundamental rule; they must be previously decided because the chemistry model, as every model, has a narrow range of validity and fits real data in a narrow range. It is not uncommon that models which fit data just in some points are adopted, by means of extrapolation laws, to figure out chemistry behaviours in ranges wider than their original validity without highlighting the errors percentage differences in these new ranges. Unfortunately this operation leads to big mistakes which are often neglected.

Experience shows, and this will be clear in the following sections, that most or almost all reduced mechanisms are tuned to predict data at high temperatures (where it is easy to obtain accurate data) but often at low temperatures, and low pressure, (i.e. 1000K-2000K and for pressures in the range between 1atm and 5atm, typical of non-adiabatic combustion) they are not accurate or do not predict ignition at all.

In general, for a semiglobal mechanism, the simplest overall reaction representing the oxidation of a conventional hydrocarbon fuel is:

\[
\text{Fuel} + n_i \text{O}_2 + (3.76N_2) \rightarrow n_2 \text{CO}_2 + n_3 \text{H}_2\text{O} + (n_i 3.76N_2)
\]

where $n_i$ are determined by the choice of fuel.

This global reaction is often a convenient way of approximating the effects of the many elementary reactions which actually occur but it overestimates the final temperature and mispredicts the overall reaction rate.

The rate expression of the single reaction is usually expressed by:

\[
k_{oc} = AT^n \exp\left(-\frac{E_a}{RT}\right)[\text{Fuel}]^a[\text{Oxider}]^b
\]

where:
- $A$ is the frequency factor which depends on how often molecules collide when all concentrations are 1mol/L and on whether the molecules are properly oriented when they collide;
- $E_a$ is the energy that must be overcome for a chemical reaction to occur (kJ/mole);
- $n$ defines the functionality rate law with temperature;
- $a$ and $b$ define the functionality rate law with fuel and oxider mass fractions;

This rate must therefore represent an appropriate average of all of the individual reaction rates involved during the reaction and this is obtained tuning the $A$, $E_a$, $n$, $a$ and $b$ variables.

3. Reaction mechanisms

The reaction mechanisms presented here are:
1. Westbrook and Dryer: 4 species and 1 reaction (Westbrook & Dryer, 1981);
2. Westbrook and Dryer: 5 species and 2 reactions (Westbrook & Dryer, 1981);
3. Minotti: 6 species and 2 reactions (Minotti et al., 2009);
4. Kee: 17 species and 58 reactions (Kee et al., 1985);
5. GRI-Mech 12: 32 species and 177 reactions (Gri-Mech 1.2, 1994; Heffington et al., 1997); These mechanisms have been compared to the predictions given by the detailed GRI-Mech 3.0 (53 species and 325 reactions (GRI-Mech 3.0, 1999; Dagaut et al., 1991)), assumed as the “reference model”, for a wide range of equivalence ratio (0.3 ≤ Φ ≤ 1.9), and at three different pressures (P=1, 3 and 5 atm).

In the following sections the ignition delay comparison and the final temperature comparison are respectively reported.

4. Comparisons – ignition delay times

The ignition delay time is the elapsed time to obtain a temperature increase, from the injection temperature, of 400K.

The ignition delay time has been compared among the five mechanisms, listed above, adopting reactants in the temperature range 1000K - 2000K and at pressure 1, 3 and 5 atm. The equivalence ratio (Φ) range tested was from Φ=0.3 to Φ=1.9 (ΔΦ=0.2), plus Φ=1.

Table 1a and Table 1b provide the ignition delay times, t_{id}, predicted by the reference detailed GRI-Mech 3.0 mechanism as function of temperature, for P=1 atm, and at Φ previously indicated (Tables 12a-12b and 23a-23b report data respectively at P=3 atm and P=5 atm).

| Reactants Temperature, K | Φ=0.3 | Φ=0.5 | Φ=0.7 | Φ=0.9 | Φ=1 |
|--------------------------|--------|--------|--------|--------|-----|
| 1000                     | 0.608  | 0.772  | 0.982  | 1.03   | 1.04|
| 1100                     | 0.111  | 0.143  | 0.131  | 0.192  | 0.202|
| 1200                     | 0.0244 | 0.0314 | 0.0331 | 0.0424 | 0.044|
| 1300                     | 0.00649| 0.00815| 0.00967| 0.011  | 0.0114|
| 1400                     | 0.00211| 0.00247| 0.00289| 0.00323| 0.00336|
| 1500                     | 0.000881| 0.000915| 0.00103| 0.00112| 0.00114|
| 1600                     | 0.000422| 0.000398| 0.000423| 0.000439| 0.000456|
| 1700                     | 0.000246| 0.000197| 0.000203| 0.000203| 0.000211|
| 1800                     | 0.000174| 0.000108| 0.000106| 0.000107| 0.000109|
| 1900                     | 0.000148| 0.000067| 0.0000638| 0.0000627| 0.0000628|
| 2000                     | 0.000139| 0.0000398| 0.0000381| 0.0000375| 0.0000377|

Table 1. a Ignition Delay, s, P=1 atm

| Reactants Temperature, K | Φ=1.1 | Φ=1.3 | Φ=1.5 | Φ=1.7 | Φ=1.9 |
|--------------------------|--------|--------|--------|--------|--------|
| 1000                     | 1.15   | 1.2    | 1.22   | 1.43   | 1.53   |
| 1100                     | 0.216  | 0.23   | 0.232  | 0.233  | 0.292  |
| 1200                     | 0.0473 | 0.0522 | 0.0524 | 0.0523 | 0.0642 |
| 1300                     | 0.0122 | 0.0134 | 0.0142 | 0.0155 | 0.0163 |
| 1400                     | 0.00355| 0.0039| 0.00425| 0.00445| 0.00433|
| 1500                     | 0.00121| 0.00127| 0.00133| 0.00143| 0.00152|
| 1600                     | 0.00044| 0.000492| 0.000525| 0.000529| 0.000533|
| 1700                     | 0.000213| 0.000221| 0.00023| 0.000236| 0.000244|
| 1800                     | 0.000111| 0.000112| 0.000112| 0.000116| 0.000112|
| 1900                     | 0.000062| 0.0000622| 0.0000623| 0.0000627| 0.0000638|
| 2000                     | 0.0000374| 0.0000376| 0.0000384| 0.0000385| 0.0000392|

Table 1. b Ignition Delay, s, P=1 atm
From Tables 1a-1b, Tables 12a-12b and Tables 23a-23b it is possible to define a reactants temperature range where reactions might be completed, that is a range in which the Damköhler number (residence time/chemical time) is less than 1. For example these tables indicate that ignition delay times vary between $8.43 \times 10^{-6}$ s and 1.54 s. Figure 1 reports the ignition delay ($t_{id}$), at $\Phi = 1$, as function of reactants temperature and for the different reaction mechanisms.

![Figure 1. $\Phi=1.0$: $t_{id}$ comparison](image)

Tables 2 to 11 show the percent differences between the $t_{id}$ predicted by GRI-Mech 3.0 and the reduced mechanisms tested (that is, GRI-Mech3.0 - Reduced Mechanism)/GRI-Mech3.0) at pressure equal to 1 atm and for all the equivalence ratios mentioned above. Negative percentages mean that the reduced mechanism overpredicts the reference. Blank spaces mean that no convergence or no ignition has been obtained at that temperature. Tables, instead of figures, have been chosen for clarity (in some cases differences are too large).

| Reactants Temperature | 32species $177$reactions | 17species $58$reactions | 6species $2$reactions | 4species $1reaction$ | 5species $2reactions$ |
|-----------------------|--------------------------|-------------------------|-----------------------|---------------------|-----------------------|
| 1000                  | 42.93%                   | -4176.32%               |                       |                     |                       |
| 1100                  | 25.86%                   | -2152.25%               |                       |                     |                       |
| 1200                  | 10.25%                   | -1400.00%               |                       |                     |                       |
| 1300                  | 0.62%                    | -1166.56%               |                       |                     |                       |
| 1400                  | -3.79%                   | -13075.36%              | -1298.10%             |                     |                       |
| 1500                  | 0.00%                    | -6347.22%               | -1534.51%             |                     |                       |
| 1600                  | -3.79%                   | -3383.41%               | -1817.06%             |                     |                       |
| 1700                  | -6.50%                   | -1822.76%               | -1900.00%             |                     |                       |
| 1800                  | -9.77%                   | -974.71%                | -1721.84%             |                     |                       |
| 1900                  | -16.22%                  | -513.51%                | -1352.70%             |                     |                       |
| 2000                  | -34.53%                  | -308.63%                | -1000.72%             |                     |                       |

Table 2. $\Phi=0.3$: $t_{id}$ % differences between reduced and reference mechanisms
### Table 3. $\Phi=0.5$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|------------|
|                       | 32species  | 17species | 6species | 4species | 5species |
|                       | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                  | 45.34%     | -576.17% |          |          |
| 1100                  | 27.97%     | -455.24% |          |          |
| 1200                  | 12.74%     | -355.41% |          |          |
| 1300                  | 1.35%      | -271.78% |          |          |
| 1400                  | -3.64%     | -275.30% |          |          |
| 1500                  | -5.36%     | -331.69% |          |          |
| 1600                  | -6.53%     | -407.54% |          |          |
| 1700                  | -8.63%     | -488.83% |          |          |
| 1800                  | -8.33%     | -572.22% |          |          |
| 1900                  | -2.69%     | -614.93% |          |          |
| 2000                  | -7.79%     | -736.68% |          |          |

### Table 4. $\Phi=0.7$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|------------|
|                       | 32species  | 17species | 6species | 4species | 5species |
|                       | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                  | 56.31%     | -125.05% |          |          |
| 1100                  | 6.87%      | -206.11% |          |          |
| 1200                  | -0.30%     | -145.92% |          |          |
| 1300                  | 1.34%      | -85.11%  | 84.59%   | 91.52%   |
| 1400                  | -4.50%     | -72.66%  | 84.15%   | 91.28%   |
| 1500                  | -1.94%     | -90.29%  | 83.98%   | 91.21%   |
| 1600                  | -7.09%     | -134.75% | 84.00%   | 91.61%   |
| 1700                  | -7.88%     | -181.28% | 84.53%   | 93.89%   |
| 1800                  | -9.43%     | -233.96% |          |          |
| 1900                  | -7.05%     | -263.64% |          |          |
| 2000                  | -9.97%     | -317.32% |          |          |

### Table 5. $\Phi=0.9$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|------------|
|                       | 32species  | 17species | 6species | 4species | 5species |
|                       | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                  | 49.13%     | -18.45%  |          |          |
| 1100                  | 33.85%     | -30.73%  |          |          |
| 1200                  | 12.03%     | -28.07%  |          |          |
| 1300                  | 5.45%      | -9.09%   | 84.82%   | 91.64%   |
| 1400                  | -5.88%     | -5.88%   | 84.43%   | 91.21%   |
| 1500                  | -5.36%     | -14.29%  | 83.13%   | 90.98%   |
| 1600                  | -10.48%    | -43.05%  | 82.44%   | 90.75%   |
| 1700                  | -12.32%    | -66.56%  | 82.32%   | 90.49%   |
| 1800                  | -13.08%    | -106.54% |          |          |
| 1900                  | -10.05%    | -129.67% |          |          |
| 2000                  | -12.00%    | -162.93% |          |          |
Table 6. $\Phi=1.0$: $\text{tid}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|----------|----------|----------|----------|----------|
|                      | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |%
| 1000                 | 44.76%      | -0.97%   | 74.66%   | 86.21%   |          |          |
| 1100                 | 27.72%      | 0.00%    | 84.60%   | 90.54%   |          |          |
| 1200                 | 9.09%       | -5.00%   | 84.05%   | 91.36%   |          |          |
| 1300                 | 1.75%       | 5.26%    | 84.74%   | 92.01%   |          |          |
| 1400                 | -2.72%      | 0.00%    | 84.88%   | 83.38%   |          |          |
| 1500                 | -1.40%      | -8828.57% | 3.57%    | 90.54%   | 84.35%   |          |
| 1600                 | -0.88%      | -7087.50% | 1.56%    | 89.84%   | 84.38%   |          |
| 1700                 | -0.53%      | -5207.02% | -5.26%   | 82.98%   | 84.47%   |          |
| 1800                 | -0.19%      | -4280.28% | -15.35%  | 85.21%   | 85.49%   |          |
| 1900                 | -0.17%      | -3255.26% | -28.95%  | 82.46%   | 84.96%   |          |
| 2000                 | -0.28%      | -2768.42% | -28.62%  | 83.55%   | 86.41%   |          |

Table 7. $\Phi=1.1$: $\text{tid}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|----------|----------|----------|----------|----------|
|                      | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |%
| 1000                 | 48.52%      | 29.30%   | 80.96%   | 90.40%   |          |          |
| 1100                 | 29.63%      | 20.37%   | 85.28%   |          |          |          |
| 1200                 | 10.99%      | 15.01%   | 84.97%   |          |          |          |
| 1300                 | 0.00%       | 22.21%   | 84.75%   | 91.64%   |          |          |
| 1400                 | -6.76%      | -8857.75% | 26.76%   | 84.51%   | 91.15%   |          |
| 1500                 | -8.26%      | -5197.52% | 22.40%   | 82.98%   | 90.66%   |          |
| 1600                 | -18.18%     | -3581.82% | -1.82%   | 80.41%   | 89.73%   |          |
| 1700                 | -12.21%     | -2252.11% | -19.72%  | 81.22%   | 90.23%   |          |
| 1800                 | -9.91%      | -1575.68% | -41.44%  | 81.89%   | 90.63%   |          |
| 1900                 | -12.68%     | -1187.32% | -63.72%  | 82.66%   | 5.14%    |          |
| 2000                 | -13.37%     | -926.74%  | -86.36%  | 83.48%   | 91.28%   |          |

Table 8. $\Phi=1.3$: $\text{tid}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|----------|----------|----------|----------|----------|
|                      | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |%
| 1000                 | 50.56%      | 51.43%   | 75.24%   | 90.40%   |          |          |
| 1100                 | 31.65%      | 44.73%   | 82.57%   | 90.84%   |          |          |
| 1200                 | 11.69%      | 40.61%   | 84.54%   | 92.07%   |          |          |
| 1300                 | 1.49%       | 43.81%   | 84.55%   | 91.72%   |          |          |
| 1400                 | -5.64%      | -8156.41% | 45.90%   | 84.38%   | 91.95%   |          |
| 1500                 | -11.81%     | -5002.36% | 41.65%   | 83.31%   | 90.24%   |          |
| 1600                 | -11.99%     | -3213.01% | 29.67%   | 80.67%   | 89.76%   |          |
| 1700                 | -13.12%     | -2171.49% | 11.31%   | 80.90%   | 90.41%   |          |
| 1800                 | -12.50%     | -1578.57% | -7.14%   | 81.43%   | 90.00%   |          |
| 1900                 | -14.61%     | -1203.37% | -25.52%  | 80.74%   | 89.70%   |          |
| 2000                 | -14.63%     | -937.23%  | -42.02%  | 81.73%   | 90.29%   |          |
### Table 9. $\Phi=1.5$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 48.69%     | 58.28%     | 73.93%     | 90.00%    |           |          |
| 1100                  | 21.98%     | 56.03%     | 82.03%     | 90.56%    |           |          |
| 1200                  | 4.58%      | 51.53%     | 95.42%     | 92.02%    |           |          |
| 1300                  | -2.82%     | 53.87%     | 84.37%     | 91.62%    |           |          |
| 1400                  | -5.88%     | -7547.06%  | 58.12%     | 83.72%    | 92.54%    |          |
| 1500                  | -13.53%    | -4817.29%  | 53.61%     | 80.98%    | 89.92%    |          |
| 1600                  | -11.05%    | -3023.81%  | 45.52%     | 80.19%    | 89.70%    |          |
| 1700                  | -13.04%    | -2113.04%  | 30.87%     | 79.30%    | 90.35%    |          |
| 1800                  | -16.96%    | -1596.43%  | 13.21%     | 80.63%    | 77.59%    |          |
| 1900                  | -17.98%    | -1219.42%  | -1.61%     | 81.86%    | 95.92%    |          |
| 2000                  | -14.84%    | -931.25%   | -12.50%    | 89.97%    | 93.46%    |          |

### Table 10. $\Phi=1.7$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 49.30%     | 71.26%     | 77.62%     | 91.40%    |           |          |
| 1100                  | 16.88%     | 60.69%     | 81.86%     | 90.43%    |           |          |
| 1200                  | -64.71%    | 31.58%     | 71.73%     | 84.33%    |           |          |
| 1300                  | -1.29%     | 63.48%     | 84.45%     | 91.68%    |           |          |
| 1400                  | -8.09%     | -7270.79%  | 64.94%     | 83.96%    | 91.01%    |          |
| 1500                  | -12.59%    | -4508.39%  | 63.08%     | 80.77%    | 89.86%    |          |
| 1600                  | -16.45%    | -3019.09%  | 54.06%     | 78.64%    | 88.62%    |          |
| 1700                  | -14.83%    | -2069.49%  | 42.37%     | 78.22%    | 88.98%    |          |
| 1800                  | -31.90%    | -1555.17%  | 29.48%     | 79.05%    | 89.91%    |          |
| 1900                  | -20.41%    | -1225.36%  | 15.15%     | 77.19%    | 87.93%    |          |
| 2000                  | -17.14%    | -944.16%   | 5.45%      | 78.70%    | 88.83%    |          |

### Table 11. $\Phi=1.9$: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 52.22%     | 79.28%     | 78.95%     | 91.90%    |           |          |
| 1100                  | 30.82%     | 75.45%     | 82.36%     | 92.40%    |           |          |
| 1200                  | 11.06%     | 70.25%     | 84.27%     | 91.98%    |           |          |
| 1300                  | -3.07%     | 69.14%     | 83.99%     | 91.60%    |           |          |
| 1400                  | -18.24%    | -7544.34%  | 68.13%     | 81.27%    | 90.12%    |          |
| 1500                  | -12.50%    | -4268.42%  | 69.01%     | 80.53%    | 89.74%    |          |
| 1600                  | -17.82%    | -3014.45%  | 60.23%     | 77.11%    | 88.16%    |          |
| 1700                  | -15.57%    | -2002.46%  | 52.87%     | 77.17%    | 87.70%    |          |
| 1800                  | -17.50%    | -1516.67%  | 40.92%     | 76.92%    | 90.00%    |          |
| 1900                  | -21.79%    | -1216.61%  | 27.74%     | 75.71%    | 87.21%    |          |
| 2000                  | -18.37%    | -938.27%   | 19.64%     | 77.32%    | 88.14%    |          |
Tables 2-11 above (P=1atm) show that:

- at $\Phi=0.3$ and $\Phi=0.5$ the Westbrook and Dryer mechanisms do not predict ignition at any temperature and ignite in a narrow $T$ range at $\Phi=0.7$ and $\Phi=0.9$. This is worthily since many researchers use this mechanism out of context, e.g., to predict properties of non-premixed flames.
- when the Westbrook and Dryer mechanisms ignite, the single step behaves better than the 2-step. Percentage differences are almost constant, that is 80% for the mechanism with 1 reaction and 90% for the mechanism with 2 reactions;
- the Kee mechanism (17 species and 58 reactions) starts predicting ignition only at temperatures $>1400$K and consistently overpredicts reference values (differences are 13000% at low $\Phi$);
- even though differences are significant in some $T$ range, the Minotti (6 species and 2 reactions) predicts the ‘best’ $t_{id}$ at every equivalence ratio except $\Phi=0.7$;
- Minotti predicts realistically $t_{id}$ at $\Phi=1$; in particular from 1000K to 1700K the difference is $<5\%$, sometimes even $<1\%$ and better than GRIMech 12 predictions which adopts 32 species and 177 reactions;
- the GRI-Mech 12 (32 species and 177 reactions) usually fits the reference values better than the other mechanisms;

Ignition delay times at P=3atm and P=5atm are also compared and provided. Here tables 12a-12b and 13a-13b, report the ignition delay times of the GRIMech3.0 detailed mechanism at P=3atm and P=5atm.

| Reactants | Temperature, K | $\Phi=0.3$ | $\Phi=0.5$ | $\Phi=0.7$ | $\Phi=0.9$ | $\Phi=1$ |
|-----------|---------------|------------|------------|------------|------------|----------|
| 1000      | 0.206         | 0.238      | 0.273      | 0.302      | 0.302      |
| 1100      | 0.0385        | 0.0474     | 0.0562     | 0.0632     | 0.0641     |
| 1200      | 0.00957       | 0.0114     | 0.0133     | 0.0152     | 0.0152     |
| 1300      | 0.00266       | 0.00324    | 0.00383    | 0.00433    | 0.00438    |
| 1400      | 0.000878      | 0.00104    | 0.00122    | 0.00133    | 0.00133    |
| 1500      | 0.000341      | 0.000385   | 0.000433   | 0.000479   | 0.000481   |
| 1600      | 0.000156      | 0.000163   | 0.000174   | 0.000186   | 0.000187   |
| 1700      | 0.0000822     | 0.0000767  | 0.0000808  | 0.0000836  | 0.0000838  |
| 1800      | 0.0000503     | 0.0000404  | 0.0000408  | 0.0000416  | 0.0000417  |
| 1900      | 0.0000356     | 0.0000234  | 0.0000227  | 0.0000228  | 0.0000228  |
| 2000      | 0.0000291     | 0.0000144  | 0.0000136  | 0.0000134  | 0.0000134  |

Table 12. a Ignition Delay, s, P=3atm

| Reactants | Temperature, K | $\Phi=1.1$ | $\Phi=1.3$ | $\Phi=1.5$ | $\Phi=1.7$ | $\Phi=1.9$ |
|-----------|---------------|------------|------------|------------|------------|-----------|
| 1000      | 0.332         | 0.225      | 0.401      | 0.432      | 0.462      |
| 1100      | 0.071         | 0.0641     | 0.0826     | 0.0902     | 0.0962     |
| 1200      | 0.0172        | 0.0191     | 0.0202     | 0.0221     | 0.0233     |
| 1300      | 0.00426       | 0.00591    | 0.00527    | 0.00622    | 0.00631    |
| 1400      | 0.00151       | 0.00191    | 0.00172    | 0.00185    | 0.00201    |
| 1500      | 0.000521      | 0.00066    | 0.000601   | 0.000636   | 0.000631   |
| 1600      | 0.000201      | 0.000248   | 0.000222   | 0.000235   | 0.000248   |
| 1700      | 0.0000874     | 0.000103   | 0.0000924  | 0.0000972  | 0.000102   |
| 1800      | 0.0000427     | 0.000051   | 0.0000451  | 0.0000465  | 0.0000479  |
| 1900      | 0.0000231     | 0.0000272  | 0.0000239  | 0.0000244  | 0.0000251  |
| 2000      | 0.0000135     | 0.0000159  | 0.0000139  | 0.0000141  | 0.0000143  |

Table 12. b Ignition Delay, s, P=3atm
Reactants Temperature, K | Φ=0.3 | Φ=0.5 | Φ=0.7 | Φ=0.9 | Φ=1
--- | --- | --- | --- | --- | ---
1000 | 0.125 | 0.134 | 0.153 | 0.17 | 0.172
1100 | 0.0234 | 0.0274 | 0.0322 | 0.0362 | 0.0382
1200 | 0.00577 | 0.00682 | 0.00827 | 0.00923 | 0.00982
1300 | 0.0017 | 0.00204 | 0.00242 | 0.00272 | 0.00282
1400 | 0.000578 | 0.000685 | 0.000738 | 0.000886 | 0.000921
1500 | 0.000228 | 0.000255 | 0.000285 | 0.000316 | 0.000331
1600 | 0.000101 | 0.000106 | 0.000114 | 0.000123 | 0.000131
1700 | 0.0000519 | 0.0000504 | 0.0000529 | 0.0000555 | 0.0000571
1800 | 0.0000303 | 0.0000262 | 0.0000264 | 0.0000272 | 0.0000275
1900 | 0.0000202 | 0.0000147 | 0.0000145 | 0.0000146 | 0.0000147
2000 | 0.0000154 | 0.00000893 | 0.00000868 | 0.00000843 | 0.00000861

Table 13. a Ignition Delay, s, P=5atm

Reactants Temperature, K | Φ=1.1 | Φ=1.3 | Φ=1.5 | Φ=1.7 | Φ=1.9
--- | --- | --- | --- | --- | ---
1000 | 0.182 | 0.202 | 0.213 | 0.233 | 0.248
1100 | 0.0402 | 0.044 | 0.0472 | 0.0512 | 0.0543
1200 | 0.0102 | 0.0112 | 0.0122 | 0.0132 | 0.0141
1300 | 0.00301 | 0.00328 | 0.00352 | 0.00381 | 0.00402
1400 | 0.000975 | 0.00102 | 0.00112 | 0.00122 | 0.00128
1500 | 0.000342 | 0.000371 | 0.000391 | 0.000422 | 0.00043
1600 | 0.000132 | 0.000142 | 0.00013 | 0.00016 | 0.000166
1700 | 0.0000582 | 0.0000612 | 0.0000623 | 0.0000665 | 0.000068
1800 | 0.000028 | 0.0000289 | 0.0000298 | 0.0000308 | 0.0000318
1900 | 0.0000149 | 0.0000151 | 0.0000154 | 0.0000159 | 0.0000163
2000 | 0.00000845 | 0.00000872 | 0.00000877 | 0.00000902 | 0.00000916

Table 13. b Ignition Delay, s, P=5atm

Tables A1-A10 and A11-A20 (in the appendix) report, respectively, the percentage differences at P=3atm and at P=5atm.

Tables A1-A20 show that reaction mechanisms worsen their accuracy increasing the operating pressure to P=3atm and P=5 atm, in fact:
- the 1-step and 2-step Westbrook and Dryer mechanisms start igniting only at Φ= 1.0 and Φ=1.1, respectively, both for P=3atm and P=5atm (at P=1atm ignition occurs for Φ>0.7).
- the Kee mechanism predicts ignition only at T > 1500K, both at P=3atm and P=5atm, (at P=1atm the minimum temperature is 1400K), and it consistently overpredicts reference values;
- the Minotti ‘ignites’ at all Φ, both for P=3atm and P=5atm, behaves worse than at 1atm;
- the single-step Westbrook and Dryer mechanism when it ignites, behaves better than the two-step and the Minotti mechanism;
- the GRI-Mech 12 usually fits the reference values better than the other mechanisms.

5. Comparison – equilibrium temperatures

A parallel comparison was carried out for the equilibrium temperatures predictions. Table 14a-14b report the temperature predicted by the GRI-Mech 3.0, when equilibrium is reached, as a function of Φ and reactants temperature, at P=1atm.
Figures 2 to 11 report equilibrium temperature at $P=1$, from $\Phi=0.3$ to $\Phi=1.9$ as function of reactants temperature.
Simulations were carried out up to one hundred times the ignition delay.

| Reactants Temperature, K | $\Phi=0.3$ | $\Phi=0.5$ | $\Phi=0.7$ | $\Phi=0.9$ | $\Phi=1$ |
|-------------------------|------------|------------|------------|------------|------------|
| 1000                    | 1682       | 2043       | 2325       | 2497       | 2517       |
| 1100                    | 1774       | 2123       | 2387       | 2541       | 2560       |
| 1200                    | 1866       | 2201       | 2445       | 2584       | 2601       |
| 1300                    | 1956       | 2276       | 2499       | 2626       | 2641       |
| 1400                    | 2046       | 2347       | 2551       | 2665       | 2680       |
| 1500                    | 2135       | 2417       | 2602       | 2704       | 2717       |
| 1600                    | 2218       | 2482       | 2650       | 2742       | 2753       |
| 1700                    | 2298       | 2542       | 2689       | 2777       | 2789       |
| 1800                    | 2373       | 2591       | 2730       | 2812       | 2823       |
| 1900                    | 2445       | 2643       | 2770       | 2845       | 2856       |
| 2000                    | 2507       | 2692       | 2808       | 2878       | 2888       |

Table 14. a Temperature at Steady State, K, $P=1$atm

| Reactants Temperature, K | $\Phi=1.1$ | $\Phi=1.3$ | $\Phi=1.5$ | $\Phi=1.7$ | $\Phi=1.9$ |
|-------------------------|------------|------------|------------|------------|------------|
| 1000                    | 2559       | 2516       | 2516       | 2287       | 2165       |
| 1100                    | 2600       | 2570       | 2570       | 2364       | 2247       |
| 1200                    | 2640       | 2621       | 2621       | 2438       | 2327       |
| 1300                    | 2499       | 2626       | 2602       | 2508       | 2405       |
| 1400                    | 2551       | 2665       | 2658       | 2574       | 2479       |
| 1500                    | 2602       | 2704       | 2709       | 2636       | 2549       |
| 1600                    | 2650       | 2742       | 2756       | 2693       | 2614       |
| 1700                    | 2689       | 2777       | 2799       | 2745       | 2675       |
| 1800                    | 2853       | 2861       | 2861       | 2893       | 2793       |
| 1900                    | 2885       | 2894       | 2877       | 2838       | 2783       |
| 2000                    | 2915       | 2926       | 2913       | 2879       | 2831       |

Table 14. b Temperature at Steady State, K, $P=1$atm

Fig. 2. $\Phi=0.3$, $P=1$atm, temperature
Fig. 3. $\Phi=0.5$, $P=1$ atm, temperature

Fig. 4. $\Phi=0.7$, $P=1$ atm, temperature

Fig. 5. $\Phi=0.9$, $P=1$ atm, temperature
Fig. 6. $\Phi=1.0$, $P=1\text{atm}$, temperature

Fig. 7. $\Phi=1.1$, $P=1\text{atm}$, temperature

Fig. 8. $\Phi=1.3$, $P=1\text{atm}$, temperature
Fig. 9. $\Phi=1.5$, $P=1\text{atm}$, temperature

Fig. 10. $\Phi=1.7$, $P=1\text{atm}$, temperature

Fig. 11. $\Phi=1.9$, $P=1\text{atm}$, temperature
Above results indicate that:

- Minotti predicted temperatures are always much closer to reference than using the two Westbrook and Dryer mechanisms (when they ignite);

- Minotti mechanism is much more accurate than the other semiglobal W&D mechanisms; accuracy (in percentage difference) is at least of the double, but for some temperature and equivalence ration ranges it reaches grade of accuracy of 4 times better;

- unlike the ignition delay times, mechanisms with large number of reactions and species predict temperatures, when they ignite, with always higher accuracy than reduced mechanisms (those predicted with the Kee mechanism, differently from the ignition delay, are close to reference);

- the GRI-Mech 12 usually fits the reference values better than the other mechanisms.

Tables 15a-15b and 16a-16b provide the Temperature at Steady State at pressures equal to 3 and 5atm predicted by the GRI-Mech3.0 (detailed mechanism). Figures A1-A10 and A11-A20 (in the Appendix) report equilibrium temperature, respectively, at P=3atm and at P=5atm, from Φ=0.3 to Φ=1.9 as function of reactants temperature.

| Reactants Temperature, K | Φ=0.3 | Φ=0.5 | Φ=0.7 | Φ=0.9 | Φ=1 |
|--------------------------|-------|-------|-------|-------|-----|
| 1000                     | 1682  | 2047  | 2346  | 2543  | 2549|
| 1100                     | 1774  | 2130  | 2413  | 2593  | 2598|
| 1200                     | 1866  | 2210  | 2477  | 2641  | 2646|
| 1300                     | 1958  | 2289  | 2538  | 2687  | 2692|
| 1400                     | 2051  | 2366  | 2596  | 2732  | 2736|
| 1500                     | 2140  | 2438  | 2651  | 2775  | 2779|
| 1600                     | 2230  | 2511  | 2703  | 2817  | 2821|
| 1700                     | 2315  | 2578  | 2753  | 2858  | 2861|
| 1800                     | 2397  | 2651  | 2800  | 2898  | 2901|
| 1900                     | 2475  | 2705  | 2847  | 2936  | 2939|
| 2000                     | 2545  | 2756  | 2890  | 2973  | 2976|

Table 15. a Temperature at Steady State, K, P=3atm

| Reactants Temperature, K | Φ=1.1 | Φ=1.3 | Φ=1.5 | Φ=1.7 | Φ=1.9 |
|--------------------------|-------|-------|-------|-------|-------|
| 1000                     | 2611  | 2554  | 2426  | 2296  | 2170  |
| 1100                     | 2659  | 2619  | 2501  | 2377  | 2255  |
| 1200                     | 2704  | 2680  | 2573  | 2457  | 2339  |
| 1300                     | 2748  | 2737  | 2642  | 2534  | 2422  |
| 1400                     | 2790  | 2790  | 2706  | 2608  | 2502  |
| 1500                     | 2831  | 2839  | 2766  | 2678  | 2580  |
| 1600                     | 2870  | 2885  | 2822  | 2744  | 2654  |
| 1700                     | 2909  | 2928  | 2873  | 2806  | 2723  |
| 1800                     | 2946  | 2969  | 2922  | 2863  | 2789  |
| 1900                     | 2982  | 3008  | 2967  | 2916  | 2850  |
| 2000                     | 3017  | 3045  | 3009  | 2966  | 2907  |

Table 15. b Temperature at Steady State, K, P=3atm
Figures A1-A20 (in the appendix) show that all reaction mechanisms, but the Minotti one, worse their accuracy increasing the operating pressure to $P=3\text{atm}$ and $P=5\text{atm}$, in fact:

- the 1-step and 2-step Westbrook and Dryer mechanisms do not predict ignition for wide ranges of equivalence ratio both for $P=3\text{atm}$ and $P=5\text{atm}$ (at $P=1\text{atm}$ ignition occurs for $\Phi>0.7$); moreover the 2-step mechanism is slightly more accurate than the 1-step mechanism;

- the Minotti ‘ignites’ at all $\Phi$, and it holds its overall level of accuracy and it behaves better than at $P=1\text{atm}$ for some ranges of temperature and equivalence ratio;

- Minotti mechanism is much more accurate than the other semiglobal W&D mechanisms; accuracy (in percentage difference) is at least of the double, but, for some temperature and equivalence ratio ranges, it reaches grade of accuracy of 100 times better.

- the Kee mechanism predicts ignition only at $T > 1500\text{K}$, both at $P=3\text{atm}$ and $P=5\text{atm}$, (at $P=1\text{atm}$ the minimum temperature is $1400\text{K}$), and it predicts values with high level of accuracy;

- the GRI-Mech 12 usually fits the reference values better than the other mechanisms.

---

| Reactants Temperature, K | $\Phi=0.3$ | $\Phi=0.5$ | $\Phi=0.7$ | $\Phi=0.9$ | $\Phi=1$ |
|--------------------------|------------|------------|------------|------------|-----------|
| 1000                     | 1682       | 2048       | 2353       | 2562       | 2618      |
| 1100                     | 1774       | 2131       | 2423       | 2615       | 2666      |
| 1200                     | 1867       | 2214       | 2490       | 2665       | 2713      |
| 1300                     | 1960       | 2294       | 2554       | 2714       | 2758      |
| 1400                     | 2052       | 2372       | 2615       | 2761       | 2802      |
| 1500                     | 2144       | 2447       | 2673       | 2807       | 2845      |
| 1600                     | 2234       | 2521       | 2728       | 2851       | 2887      |
| 1700                     | 2321       | 2590       | 2780       | 2894       | 2928      |
| 1800                     | 2404       | 2655       | 2831       | 2936       | 2968      |
| 1900                     | 2483       | 2722       | 2878       | 2977       | 3007      |
| 2000                     | 2561       | 2778       | 2924       | 3016       | 3045      |

Table 16. a Temperature at Steady State, K, $P=5\text{atm}$

| Reactants Temperature, K | $\Phi=1.1$ | $\Phi=1.3$ | $\Phi=1.5$ | $\Phi=1.7$ | $\Phi=1.9$ |
|--------------------------|------------|------------|------------|------------|------------|
| 1000                     | 2634       | 2560       | 2431       | 2299       | 2171       |
| 1100                     | 2684       | 2626       | 2509       | 2380       | 2257       |
| 1200                     | 2732       | 2690       | 2584       | 2463       | 2343       |
| 1300                     | 2778       | 2749       | 2656       | 2543       | 2427       |
| 1400                     | 2823       | 2804       | 2725       | 2620       | 2511       |
| 1500                     | 2866       | 2855       | 2789       | 2649       | 2591       |
| 1600                     | 2908       | 2904       | 2849       | 2764       | 2668       |
| 1700                     | 2949       | 2950       | 2905       | 2830       | 2742       |
| 1800                     | 2988       | 2993       | 2957       | 2892       | 2812       |
| 1900                     | 3026       | 3034       | 3006       | 2949       | 2877       |
| 2000                     | 3064       | 3074       | 3051       | 3003       | 2938       |

Table 16. b Temperature at Steady State, K, $P=5\text{atm}$
6. Conclusions

Current studies on space missions and on micro-combustion, also for Micro-Rockets applications, gave the cue for the present work. This chapter focuses its attention on some of the most important points concerning with reaction mechanisms and, at the same time, five mechanisms are presented, analysed and compared; they deal with hydrocarbon oxidation, in particular methane. Comparison is carried out for a wide range of equivalence ratios \(0.3 \leq \Phi \leq 1.9\), temperatures \((1000\text{K}-2000\text{K})\) and pressure \((1 \leq P [\text{atm}] \leq 5)\), adopting as benchmark the detailed GRIMech3.0 reference mechanism, which adopts 55 species and 325 reactions. This study is important because analyses the mechanisms effectiveness in predicting ignition in good agreement with detailed kinetics calculations with low temperature and low pressures ignition ranges.

These ranges are typical of non-adiabatic combustion and, unfortunately, reduced mechanisms found in literature often fail to predict realistic delay times and equilibrium flame temperatures under these conditions but are usually adopted without a previous validity study. In applications where the flame temperature is lower or much lower than adiabatic, realism and accuracy are indeed critical.

Some general results may be summarised. Among the semiglobal mechanisms, the Minotti 2-step reduced mechanism is well suited for low temperature flames, that is, in devices where heat losses, e.g., through non-adiabatic walls, are not negligible. Results are in some cases surprising, showing this mechanism predicts, in some ranges, ignition delay times and equilibrium temperatures better than other reduced and even detailed mechanisms, showing also that it ‘ignites’ at all \(P\) and \(\Phi\).

Thus it is not always true that including larger numbers of species and reactions predict ignition delays better, in fact there are wide ranges of \(T\) and \(\Phi\) in which the Kee mechanism (17 species and 58 reactions) does not ignite and/or is less accurate than other simplified mechanisms. The Westbrook and Dryer mechanisms ignite only at particular equivalence ratios and at particular reactants temperature.

As for the effect of pressure, at 1atm the Minotti mechanism predicts ignition delays times always more accurately than the other reduced mechanisms, except at \(\Phi=0.7\) and for \(1500<T [\text{K}]<1700\), where the two Westbrook and Dryer mechanisms behave better. At 3 and 5 atm the behavior is in general the same.

The comparison among predicted equilibrium temperature has shown that mechanisms with high number of species, predict final (stationary) temperatures, when they ignite, better than mechanism with a lower number of species, as it is expected since simpler mechanism cannot include radicals. Comparisons are then meaningful only between mechanisms with similar numbers of species and reactions.

This said, Minotti one is always much more accurate than the two Westbrook and Dryer mechanisms.

To conclude the Minotti mechanism is appropriate for preliminary combustion studies in all the devices that operate at low temperature and pressure, as it combines high accuracy and reliability with ease of implementation and a modest computational effort.

7. Appendix

Ignition delay, \(P=3\text{atm}\) and \(P=5\text{atm}\), comparison
### Table A1. P=3atm, Φ=0.3: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|-------------|
|                       | 32species | 17species | 6species | 4species | 5species |
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 29.61%     | -2919.42% |
| 1100                  | 7.01%      | -858.44%  |
| 1200                  | 0.00%      | -377.53%  |
| 1300                  | -10.90%    | -217.29%  |
| 1400                  | -11.50%    | -172.21%  |
| 1500                  | -9.97%     | -6996.77% |
| 1600                  | -8.33%     | -3592.31% |
| 1700                  | -8.03%     | -2004.62% |
| 1800                  | -9.34%     | -1237.97% |
| 1900                  | -12.08%    | -686.52%  |
| 2000                  | -17.18%    | -405.15%  |

### Table A2. P=3atm, Φ=0.5: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|-------------|
|                       | 32species | 17species | 6species | 4species | 5species |
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 31.51%     | -144.54% |
| 1100                  | 10.97%     | -71.31%  |
| 1200                  | -7.02%     | -34.21%  |
| 1300                  | -12.04%    | -1.85%   |
| 1400                  | -11.54%    | 18.46%   |
| 1500                  | -12.47%    | -6731.17%|
| 1600                  | -7.98%     | -3703.68%|
| 1700                  | -9.13%     | -2272.88%|
| 1800                  | -8.91%     | -1503.96%|
| 1900                  | -8.12%     | -1053.85%|
| 2000                  | -7.64%     | -781.94% |

### Table A3. P=3atm, Φ=0.7: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|-----------------------|-------------|
|                       | 32species | 17species | 6species | 4species | 5species |
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 52.75%     | 31.14%    |
| 1100                  | 23.67%     | -71.31%  |
| 1200                  | -6.02%     | -34.21%  |
| 1300                  | -12.53%    | 18.46%   |
| 1400                  | -14.75%    | -6731.17%|
| 1500                  | -13.86%    | -3703.68%|
| 1600                  | -11.49%    | -2272.88%|
| 1700                  | -6.68%     | -1503.96%|
| 1800                  | -10.78%    | -1053.85%|
| 1900                  | -11.45%    | -781.94% |
| 2000                  | -11.76%    | -781.94% |

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## Table A4. P=3atm, Φ=0.9: t\text{id} % differences between reduced and reference mechanisms

| Reactants Temperature | 32species | 17species | 6species | 4species | 5species |
|-----------------------|-----------|-----------|----------|----------|----------|
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 58.28%     | 69.83%    | 68.20%   |           |          |
| 1100                  | 17.25%     | 71.91%    | 71.36%   |           |          |
| 1200                  | 0.00%      | 74.59%    |          |           |          |
| 1300                  | -11.55%    |           |          |           |          |
| 1400                  | -15.04%    |           |          |           |          |
| 1500                  | -15.24%    | -5829.02% | 76.62%   |           |          |
| 1600                  | -14.52%    | -3491.40% | 75.32%   |           |          |
| 1700                  | -11.48%    | -2220.57% | 71.53%   |           |          |
| 1800                  | -12.98%    | -1544.23% | 65.63%   |           |          |
| 1900                  | -13.16%    | -1145.61% | 59.34%   |           |          |
| 2000                  | -13.43%    | -892.54%  | 52.84%   |           |          |

## Table A5. P=3atm, Φ=1.0: t\text{id} % differences between reduced and reference mechanisms

| Reactants Temperature | 32species | 17species | 6species | 4species | 5species |
|-----------------------|-----------|-----------|----------|----------|----------|
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 36.42%     | 90.66%    | 67.86%   |           |          |
| 1100                  | 15.60%     | 72.17%    |          |           |          |
| 1200                  | 0.00%      | 71.92%    |          |           |          |
| 1300                  | -12.10%    |           |          |           |          |
| 1400                  | -19.55%    |           |          |           |          |
| 1500                  | -14.76%    | -5804.37% | 77.13%   |           |          |
| 1600                  | -13.90%    | -3477.54% | 75.83%   |           |          |
| 1700                  | -11.34%    | -2215.04% | 72.08%   |           |          |
| 1800                  | -12.95%    | -1542.69% | 66.19%   |           |          |
| 1900                  | -13.16%    | -1145.61% | 60.04%   |           |          |
| 2000                  | -13.43%    | -892.54%  | 53.66%   |           |          |

## Table A6. P=3atm, Φ=1.1: t\text{id} % differences between reduced and reference mechanisms

| Reactants Temperature | 32species | 17species | 6species | 4species | 5species |
|-----------------------|-----------|-----------|----------|----------|----------|
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 36.14%     | 81.72%    | 58.66%   |           |          |
| 1100                  | 26.34%     | 81.57%    | 58.66%   |           |          |
| 1200                  | 0.00%      | 72.07%    |          |           |          |
| 1300                  | -22.54%    |           |          |           |          |
| 1400                  | -13.91%    |           |          |           |          |
| 1500                  | -17.85%    | -5466.22% | 79.08%   |           |          |
| 1600                  | -12.94%    | -3302.99% | 79.55%   |           |          |
| 1700                  | -14.42%    | -2165.45% | 76.84%   |           |          |
| 1800                  | -14.75%    | -1527.63% | 75.88%   |           |          |
| 1900                  | -14.29%    | -1151.08% | 75.36%   |           |          |
| 2000                  | -14.07%    | -900.00%  | 77.04%   |           |          |
### Table A7. P=3atm, Φ=1.3: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 37.85%     | 88.65%    | 16.85%   | 58.29%   |
| 1100                  |            | 11.59%     | 86.07%    | 43.03%   | 70.90%   |
| 1200                  |            | 0.00%      | 88.59%    | 57.75%   | 78.59%   |
| 1300                  | -13.00%    | 86.25%     | 60.99%    | 80.69%   |
| 1400                  | -17.90%    | 86.42%     | 62.41%    | 80.86%   |
| 1500                  | -17.65%    | -5176.29%  | 87.65%    | 58.65%   | 79.14%   |
| 1600                  | -16.98%    | -3187.74%  | 87.26%    | 55.14%   | 77.36%   |
| 1700                  | -12.94%    | -2114.91%  | 85.75%    | 53.73%   | 75.33%   |
| 1800                  | -16.17%    | -1517.31%  | 82.07%    | 49.43%   | 74.26%   |
| 1900                  | -16.24%    | -1156.41%  | 78.46%    | 48.72%   | 74.02%   |
| 2000                  | -16.06%    | -907.30%   | 75.04%    | 49.85%   | 75.33%   |

### Table A8. P=3atm, Φ=1.5: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 43.64%     | 92.19%    | 17.46%   | 60.19%   |
| 1100                  |            | 24.33%     | 90.24%    | 49.52%   | 73.61%   |
| 1200                  |            | 0.00%      | 89.46%    | 58.12%   | 79.41%   |
| 1300                  | -18.22%    | 88.35%     | 57.87%    | 78.94%   |
| 1400                  | -17.44%    | 91.92%     | 59.77%    | 81.69%   |
| 1500                  | -18.80%    | -4908.32%  | 90.25%    | 64.23%   | 80.70%   |
| 1600                  | -18.47%    | -3093.69%  | 89.95%    | 53.15%   | 77.07%   |
| 1700                  | -20.13%    | -2118.61%  | 88.10%    | 48.48%   | 76.84%   |
| 1800                  | -17.74%    | -1496.45%  | 85.83%    | 46.12%   | 72.73%   |
| 1900                  | -17.57%    | -1151.05%  | 82.89%    | 45.19%   | 72.43%   |
| 2000                  | -17.27%    | -907.19%   | 80.14%    | 45.97%   | 72.88%   |

### Table A9. P=3atm, Φ=1.7: $t_{id}$ % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 41.67%     | 94.93%    | 18.75%   | 60.19%   |
| 1100                  |            | 19.84%     | 97.02%    | 53.55%   | 75.61%   |
| 1200                  |            | 4.07%      | 94.48%    | 58.69%   | 81.09%   |
| 1300                  | -9.49%     | 91.72%     | 65.11%    | 80.71%   |
| 1400                  | -19.46%    | 93.19%     | 61.41%    | 82.49%   |
| 1500                  | -19.50%    | -4711.32%  | 91.71%    | 64.47%   | 78.30%   |
| 1600                  | -19.57%    | -2959.57%  | 91.70%    | 51.91%   | 76.21%   |
| 1700                  | -20.37%    | -2039.92%  | 90.77%    | 47.12%   | 75.93%   |
| 1800                  | -18.92%    | -1469.89%  | 88.39%    | 43.01%   | 71.40%   |
| 1900                  | -19.26%    | -1141.80%  | 85.94%    | 41.39%   | 70.66%   |
| 2000                  | -18.44%    | -914.18%   | 83.48%    | 41.84%   | 70.92%   |
### Kinetic Mechanisms for Aerospace Applications at Low Pressure and Temperature, Validity Ranges and Comparison

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 41.13%     | 95.32%    | 17.53%   | 59.31%   |
| 1100                  |            | 19.85%     | 94.66%    | 46.47%   | 72.87%   |
| 1200                  |            | 0.43%      | 94.81%    | 56.65%   | 78.11%   |
| 1300                  |            | -14.90%    | 93.34%    | 58.80%   | 79.40%   |
| 1400                  |            | -14.93%    | -8009.45% | 93.83%   | 60.05%   | 79.90%   |
| 1500                  |            | -28.68%    | -4812.84% | 95.28%   | 53.09%   | 76.55%   |
| 1600                  |            | -19.76%    | -2839.52% | 93.35%   | 50.81%   | 75.56%   |
| 1700                  |            | -19.61%    | -1958.82% | 93.17%   | 45.39%   | 73.53%   |
| 1800                  |            | -20.25%    | -1444.89% | 90.21%   | 40.29%   | 70.15%   |
| 1900                  |            | -19.92%    | -1127.09% | 88.09%   | 38.25%   | 69.28%   |
| 2000                  |            | -20.28%    | -913.99%  | 85.87%   | 37.83%   | 69.37%   |

Table A10. P=3atm, Φ=1.9: tid % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 23.60%     | -3020.00% | -32.02%  |
| 1100                  |            | -0.43%     | -652.14%  | -49.50%  |
| 1200                  |            | -13.69%    | -225.82%  | -71.10%  |
| 1300                  |            | -20.00%    | -87.65%   | -87.46%  |
| 1400                  |            | -17.47%    | -39.45%   | -89.60%  |
| 1500                  |            | -13.16%    | -7838.60% | -75.32%  |
| 1600                  |            | -9.90%     | -3919.80% | -57.14%  |
| 1700                  |            | -8.67%     | -2115.80% | -40.29%  |
| 1800                  |            | -9.24%     | -1236.63% | -34.15%  |
| 1900                  |            | -10.89%    | -746.53%  | -34.15%  |
| 2000                  |            | -13.64%    | -452.60%  | -34.15%  |

Table A11. P=5atm, Φ=0.3: tid % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|-----------------------|------------|-----------|-----------|----------|----------|----------|
|                       |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  |            | 23.13%     | -80.60%   | -780.18% |
| 1100                  |            | 0.73%      | -9.85%    | 34.15%   |
| 1200                  |            | -15.98%    | 20.53%    | 55.47%   |
| 1300                  |            | -19.12%    | 40.20%    | 55.47%   |
| 1400                  |            | -20.15%    | 55.47%    | 55.47%   |
| 1500                  |            | -16.86%    | -7664.71% | 62.31%   |
| 1600                  |            | -16.04%    | -4098.11% | 61.60%   |
| 1700                  |            | -10.71%    | -2360.32% | 57.14%   |
| 1800                  |            | -9.54%     | -1518.32% | 50.00%   |
| 1900                  |            | -10.88%    | -1063.27% | 41.63%   |
| 2000                  |            | -9.07%     | -780.18%  | 34.15%   |

Table A12. P=5atm, Φ=0.5: tid % differences between reduced and reference mechanisms
| Reactants Temperature | Mechanisms |
|----------------------|------------|
|                      | 32species  | 17species | 6species | 4species | 5species |
|                      | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                 | 26.80%     | 60.13%    | 63.35%    |          |          |
| 1100                 | 0.31%      | 63.35%    | 72.91%    |          |          |
| 1200                 | -10.16%    | 73.97%    | 79.95%    |          |          |
| 1300                 | -16.94%    | 79.95%    |          |          |          |
| 1400                 | -30.08%    |          |          |          |          |
| 1500                 | -20.00%    | -7198.25%|          |          |          |
| 1600                 | -17.54%    | -4022.81%|          |          |          |
| 1700                 | -13.42%    | -2357.47%|          |          |          |
| 1800                 | -12.88%    | -1574.24%|          |          |          |
| 1900                 | -12.41%    | -1127.59%|          |          |          |
| 2000                 | -9.79%     | -836.64%  |          |          |          |

Table A13. P=5atm, Φ=0.7: t_id % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|----------------------|------------|
|                      | 32species  | 17species | 6species | 4species | 5species |
|                      | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                 | 29.65%     | 82.33%    | 83.12%    |          |          |
| 1100                 | 8.29%      | 86.89%    | 86.00%    |          |          |
| 1200                 | -10.51%    | 86.66%    |          |          |          |
| 1300                 | -18.38%    | 87.16%    |          |          |          |
| 1400                 | -16.25%    | 87.85%    |          |          |          |
| 1500                 | -20.89%    | -6703.80%|          |          |          |
| 1600                 | -17.89%    | -3859.35%|          |          |          |
| 1700                 | -15.68%    | -2332.43%|          |          |          |
| 1800                 | -14.34%    | -1576.47%|          |          |          |
| 1900                 | -14.38%    | -1153.42%|          |          |          |
| 2000                 | -15.90%    | -892.88%  |          |          |          |

Table A14. P=5atm, Φ=0.9: t_id % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms |
|----------------------|------------|
|                      | 32species  | 17species | 6species | 4species | 5species |
|                      | 177reactions| 58reactions| 2reactions| 1reaction| 2reactions|
| 1000                 | 29.07%     | 86.34%    | 86.52%    |          |          |
| 1100                 | 8.12%      | 86.66%    |          |          |          |
| 1200                 | -3.87%     | 87.16%    |          |          |          |
| 1300                 | -20.92%    | 88.27%    |          |          |          |
| 1400                 | -21.61%    | 88.27%    |          |          |          |
| 1500                 | -21.45%    | -4866.10%|          |          |          |
| 1600                 | -16.03%    | -3678.63%|          |          |          |
| 1700                 | -16.29%    | -2299.30%|          |          |          |
| 1800                 | -16.00%    | -1580.00%|          |          |          |
| 1900                 | -15.65%    | -1158.50%|          |          |          |
| 2000                 | -14.63%    | -884.90%  |          |          |          |

Table A15. P=5atm, Φ=1.0: t_id % differences between reduced and reference mechanisms
### Table A16. P=5atm, Φ=1.1: t\(_{id}\) % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|-----------|-----------|----------|----------|----------|
|                      |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                 |            | 32.97%      | 93.46%    | -53.85%  | 27.47%   |
| 1100                 |            | 9.95%       | 89.85%    | 5.22%    | 52.74%   |
| 1200                 |            | -9.80%      | 88.92%    | 30.29%   | 68.92%   |
| 1300                 |            | -16.94%     | 91.33%    | 38.21%   | 69.83%   |
| 1400                 |            | -21.03%     | 95.11%    | 43.59%   | 73.95%   |
| 1500                 |            | -23.10%     | -6332.75% | 90.99%   | 38.30%   | 69.88%   |
| 1600                 |            | -21.97%     | -3695.45% | 91.21%   | 34.70%   | 69.09%   |
| 1700                 |            | -10.48%     | -2288.32% | 91.07%   | 31.10%   | 65.46%   |
| 1800                 |            | -16.79%     | -1571.43% | 89.57%   | 28.21%   | 63.93%   |
| 1900                 |            | 4.03%       | -1155.03% | 87.65%   | 27.52%   | 64.23%   |
| 2000                 |            | -17.87%     | -915.38%  | 85.09%   | 26.86%   | 62.72%   |

### Table A17. P=5atm, Φ=1.3: t\(_{id}\) % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|-----------|-----------|----------|----------|----------|
|                      |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                 |            | 34.65%      | 93.37%    | -51.49%  | 25.25%   |
| 1100                 |            | 11.14%      | 92.95%    | 4.55%    | 51.82%   |
| 1200                 |            | -8.04%      | 92.58%    | 27.95%   | 63.84%   |
| 1300                 |            | -18.60%     | 92.50%    | 37.80%   | 69.21%   |
| 1400                 |            | -28.43%     | 92.53%    | 40.29%   | 69.71%   |
| 1500                 |            | -14.56%     | -5964.69% | 93.34%   | 37.47%   | 69.27%   |
| 1600                 |            | 8.45%       | -3505.63% | 93.66%   | 33.03%   | 67.46%   |
| 1700                 |            | -17.65%     | -2220.26% | 93.28%   | 31.05%   | 63.89%   |
| 1800                 |            | -17.99%     | -1553.98% | 92.18%   | 22.49%   | 61.59%   |
| 1900                 |            | -17.88%     | -1164.90% | 90.40%   | 20.53%   | 60.40%   |
| 2000                 |            | -16.97%     | -905.73%  | 89.12%   | 21.22%   | 62.04%   |

### Table A18. P=5atm, Φ=1.5: t\(_{id}\) % differences between reduced and reference mechanisms

| Reactants Temperature | Mechanisms | 32species | 17species | 6species | 4species | 5species |
|----------------------|------------|-----------|-----------|----------|----------|----------|
|                      |            | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                 |            | 33.33%      | 95.12%    | -55.40%  | 24.41%   |
| 1100                 |            | 10.81%      | 95.49%    | 4.24%    | 53.18%   |
| 1200                 |            | -6.56%      | 97.86%    | 30.66%   | 65.98%   |
| 1300                 |            | -19.32%     | 94.18%    | 36.93%   | 68.18%   |
| 1400                 |            | -25.89%     | 97.54%    | 38.21%   | 71.96%   |
| 1500                 |            | -25.58%     | -5731.20% | 94.42%   | 35.29%   | 68.29%   |
| 1600                 |            | -39.69%     | -3884.73% | 96.45%   | 20.61%   | 61.37%   |
| 1700                 |            | -23.43%     | -2227.45% | 94.56%   | 23.92%   | 61.48%   |
| 1800                 |            | -19.80%     | -1537.58% | 93.83%   | 18.46%   | 59.40%   |
| 1900                 |            | -19.48%     | -1166.23% | 92.47%   | 14.94%   | 58.12%   |
| 2000                 |            | -18.59%     | -920.52%  | 91.61%   | 14.37%   | 58.15%   |
Table A19. P=5atm, Φ=1.7: \( t_{id} \) % differences between reduced and reference mechanisms

| Reactants Temperature | 32species | 17species | 6species | 4species | 5species |
|-----------------------|-----------|-----------|----------|----------|----------|
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 34.76%     | 96.42%    | -50.64%  | 90.60%   |
| 1100                  | 12.30%     | 96.11%    | 4.30%    | 52.93%   |
| 1200                  | 0.00%      | 95.83%    | 30.83%   | 68.33%   |
| 1300                  | -17.59%    | 95.54%    | 36.75%   | 68.77%   |
| 1400                  | -23.77%    | 95.48%    | 41.48%   | 74.02%   |
| 1500                  | -24.41%    | -5397.63% | 95.64%    | 46.45%   | 68.25%   |
| 1600                  | -21.25%    | -3218.75% | 95.80%    | 29.38%   | 66.06%   |
| 1700                  | -21.65%    | -2110.53% | 95.58%    | 22.71%   | 60.90%   |
| 1800                  | -21.10%    | -1510.39% | 95.00%    | 13.96%   | 57.47%   |
| 1900                  | -20.13%    | -1151.57% | 93.91%    | 10.06%   | 55.66%   |
| 2000                  | -19.73%    | -911.09%  | 93.28%    | 9.09%    | 55.21%   |

Table A20. P=5atm, Φ=1.9: \( t_{id} \) % differences between reduced and reference mechanisms

| Reactants Temperature | 32species | 17species | 6species | 4species | 5species |
|-----------------------|-----------|-----------|----------|----------|----------|
|                       | 177reactions | 58reactions | 2reactions | 1reaction | 2reactions |
| 1000                  | 34.68%     | 98.90%    | -53.63%  | 26.61%   |
| 1100                  | 13.08%     | 97.77%    | 5.16%    | 53.22%   |
| 1200                  | -0.71%     | 98.01%    | 28.37%   | 64.18%   |
| 1300                  | -17.91%    | 96.99%    | 35.32%   | 68.66%   |
| 1400                  | -25.78%    | -9821.88% | 97.76%    | 37.27%   | 69.06%   |
| 1500                  | -30.23%    | -5365.12% | 96.98%    | 32.56%   | 66.28%   |
| 1600                  | -24.70%    | -3146.99% | 97.99%    | 26.51%   | 63.73%   |
| 1700                  | -25.44%    | -2105.88% | 96.16%    | 18.09%   | 58.82%   |
| 1800                  | -22.64%    | -1484.91% | 95.75%    | 10.06%   | 55.66%   |
| 1900                  | -22.09%    | -1139.26% | 95.11%    | 4.91%    | 53.68%   |
| 2000                  | -21.18%    | -913.10%  | 94.26%    | 2.95%    | 53.06%   |

Fig. A1. Φ=0.3, P=3atm, temperature
Fig. A2. $\Phi=0.5$, $P=3$ atm, temperature

Fig. A3. $\Phi=0.7$, $P=3$ atm, temperature

Fig. A4. $\Phi=0.9$, $P=3$ atm, temperature
Fig. A5. $\Phi=1$, $P=3$ atm, temperature

Fig. A6. $\Phi=1.1$, $P=3$ atm, temperature

Fig. A7. $\Phi=1.3$, $P=3$ atm, temperature
Fig. A8. $\Phi=1.5$, $P=3$atm, temperature

Fig. A9. $\Phi=1.7$, $P=3$atm, temperature

Fig. A10. $\Phi=1.9$, $P=3$atm, temperature
Fig. A11. $\Phi=0.3$, $P=5$ atm, temperature

Fig. A12. $\Phi=0.5$, $P=5$ atm, temperature

Fig. A13. $\Phi=0.7$, $P=5$ atm, temperature
Fig. A14. $\Phi=0.9$, $P=5\text{atm}$, temperature

Fig. A15. $\Phi=1$, $P=5\text{atm}$, temperature

Fig. A16. $\Phi=1.1$, $P=5\text{atm}$, temperature
Fig. A17. $\Phi=1.3$, $P=5\text{ atm}$, temperature

Fig. A18. $\Phi=1.5$, $P=5\text{ atm}$, temperature

Fig. A19. $\Phi=1.7$, $P=5\text{ atm}$, temperature
Fig. A20. $\Phi=1.9$, $P=5\text{atm}$, temperature

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