# Supporting Information for

## Reactive symbol sequences for a model of hydrogen combustion

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## SI1. STUDIED TEMPERATURES AND DENSITIES

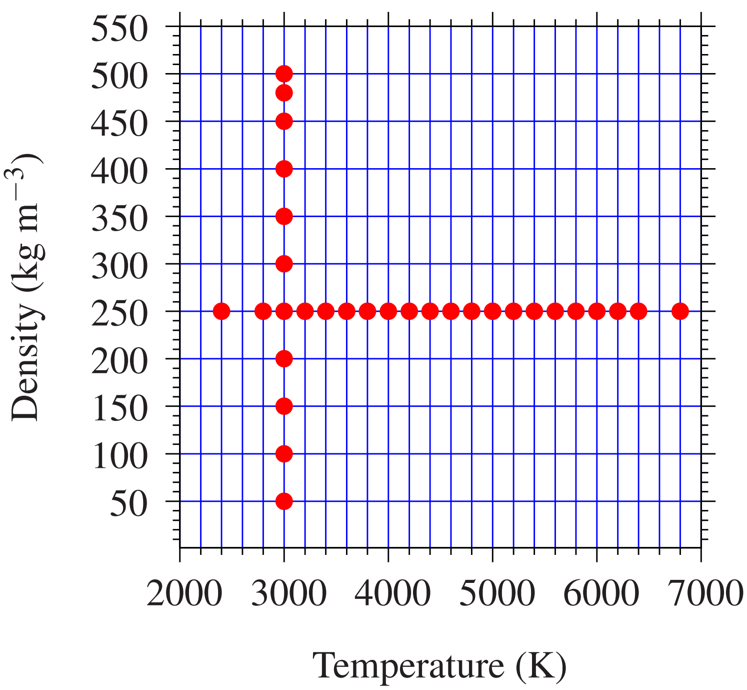


Figure 1: Studied temperatures and densities in this work.

## SI2. TIME EVOLUTION OF CHEMICAL SPECIES

Figure 2 shows the time evolution of $H_2O$ at two different temperatures of 3000 and 6000 K and a density of 250 $kg\,m^{-3}$. Increasing the temperature reduces the time to reach the maximum number of water molecules at each temperature.

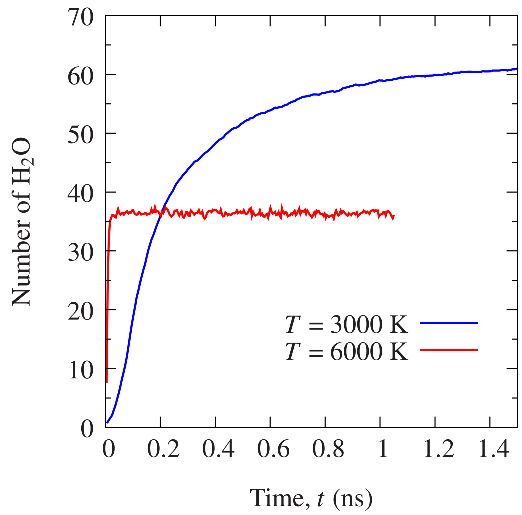


Figure 2: Time evolution of $H_2O$ number at 3000 and 6000 K and a density of 250 $kg\,m^{-3}$. Doubling the $T$ accelerates the time to "complete" the reaction, but also causes $H_2O$ dissociation which decreases the net $H_2O$ production.

The number of intermediate species at high temperatures are larger than at lower temperatures. Although all of $H_2$ and $O_2$ molecules are quickly converted to water at 6000 K, water molecules readily dissociate back to radical species. The high kinetic energy at 6000 K provides enough energy to support the existence of energetic species which are less stable at lower temperatures; see Figure 3.

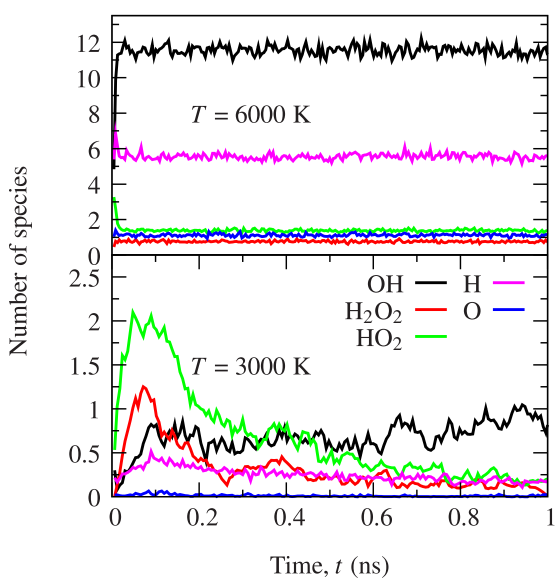


Figure 3: Time evolution of average number of intermediate species at 3000 (bottom) and 6000 K (top) and a density of 250 $kg\,m^{-3}$.

## SI3. HYDROGEN AND OXYGEN SEQUENCES

Number of steps in the trajectory of reactants to products is the length, $L$, of any sequence. The temperature dependence of the chain length probability, $P(L)$, is plotted in Figure 4 and 5 for hydrogen and oxygen sequences, respectively, for samples with density of 250 $\mathrm{kg\,m^{-3}}$. The chain length probabilities versus $L$ at 3000 K and different densities are depicted in Figure 6 and 7 for hydrogen and oxygen sequences, respectively.

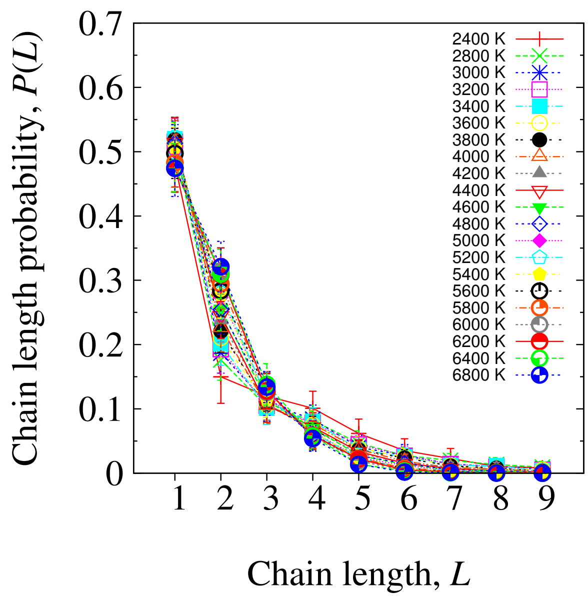


Figure 4: Chain length probability, $P(L)$, of hydrogen at a range of temperature from 2400 to 6800 K with density of 250 $\mathrm{kg\,m^{-3}}$.

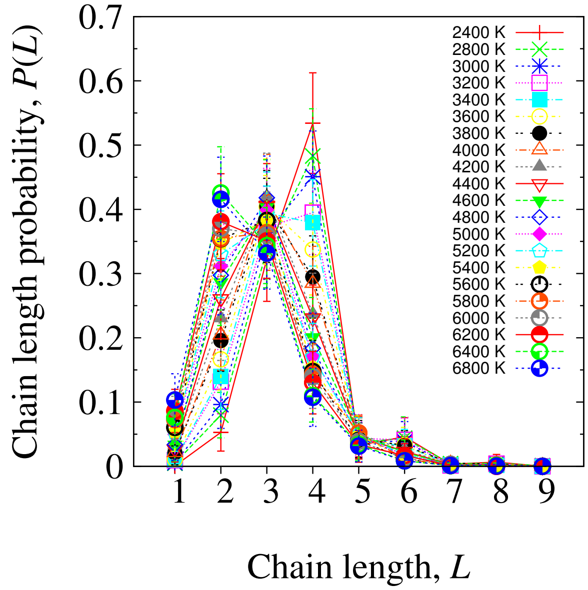


Figure 5: Chain length probability, $P(L)$, of oxygen at a range of temperature from 2400 to 6800 K with density of 250 $\mathrm{kg\,m^{-3}}$.

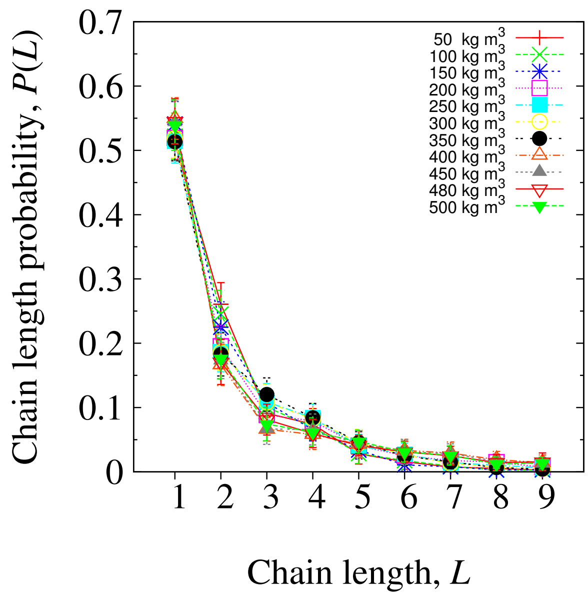


Figure 6: Chain length probability, $P(L)$, of hydrogen at 3000 K with density from 50 to 500 $\mathrm{kg\,m^{-3}}$.

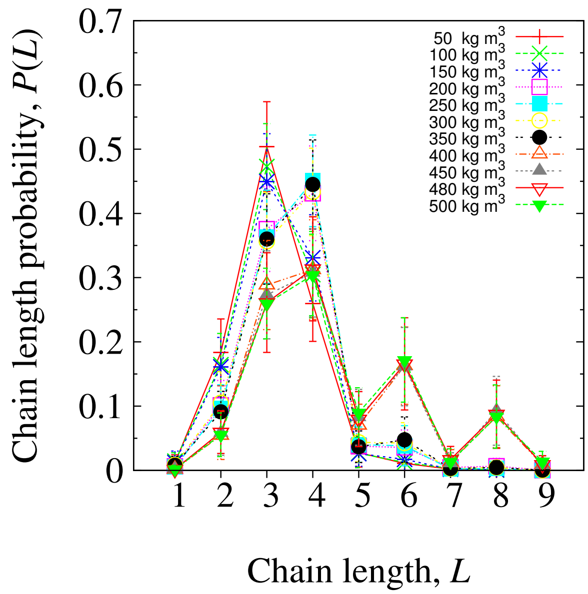


Figure 7: Chain length probability, $P(L)$, of oxygen at 3000 K with density from 50 to 500 $\mathrm{kg\,m^{-3}}$.

## SI4. Elementary reactions at $T$=3000 K and $\rho$=250 kg m$^{-3}$

| | elementary reaction | probability |
|---|---|---|
| R1 | $H_2 + OH \rightarrow H + H_2O$ | 0.2645 |
| R2 | $H + O_2 \rightarrow HO_2$ | 0.1935 |
| R3 | $H_2O_2 \rightarrow 2OH$ | 0.0838 |
| R4 | $H + HO_2 \rightarrow H_2O_2$ | 0.0774 |
| R5 | $H_2 + HO_2 \rightarrow H + H_2O_2$ | 0.0516 |
| R6 | $H + OH \rightarrow H_2O$ | 0.0451 |
| R7 | $H_2O_2 + H \rightarrow OH + H_2O$ | 0.0387 |
| R8 | $HO_2 + OH \rightarrow O_2 + H_2O$ | 0.0258 |
| R9 | $H_2 + HO_2 \rightarrow OH + H_2O$ | 0.0258 |
| R10 | $HO_2 \rightarrow O + OH$ | 0.0193 |
| R11 | $H_2 + O_2 \rightarrow H + HO_2$ | 0.0193 |
| R12 | $2HO_2 + OH \rightarrow O_2 + H + H_2O_2$ | 0.0193 |
| R13 | $O + OH \rightarrow HO_2$ | 0.0129 |
| R14 | $H + HO_2 \rightarrow 2OH$ | 0.0129 |
| R15 | $H + H_2O_2 \rightarrow OH + H_2O$ | 0.0129 |
| R16 | $H_2O_2 + OH \rightarrow HO_2 + H_2O$ | 0.0129 |
| R17 | $2OH \rightarrow H_2O_2$ | 0.0129 |
| R18 | $O_2 + OH \rightarrow O + HO_2$ | 0.0064 |
| R19 | $O_2 + H \rightarrow O + OH$ | 0.0064 |
| R20 | $HO_2 + H \rightarrow 2OH$ | 0.0064 |
| R21 | $H + HO_2 \rightarrow H_2 + O_2$ | 0.0064 |
| R22 | $H_2 + O \rightarrow H + OH$ | 0.0064 |
| R23 | $H_2O_2 \rightarrow O + H_2O$ | 0.0064 |
| R24 | $H_2 + O_2 \rightarrow O + H_2O$ | 0.0064 |
| R25 | $H_2O_2 \rightarrow H + HO_2$ | 0.0064 |
| R26 | $H_2O_2 \rightarrow H_2 + O_2$ | 0.0064 |
| R27 | $H_2 + 2O_2 \rightarrow 2HO_2$ | 0.0064 |
| R28 | $2HO_2 \rightarrow O_2 + H_2O_2$ | 0.0064 |

## SI5. Elementary reactions at $T$=6000 K and $\rho$=250 kg m$^{-3}$

| | elementary reaction | probability |
|---|---|---|
| R1 | H2 + OH → H + H2O | 0.2272 |
| R2 | H + O2 → HO2 | 0.1439 |
| R3 | H + OH → H2O | 0.1439 |
| R4 | O2 + H → O + OH | 0.0530 |
| R5 | H2 + O → H + OH | 0.0530 |
| R6 | HO2 → O + OH | 0.0454 |
| R7 | H2 + O → H2O | 0.0378 |
| R8 | H2O2 → 2OH | 0.0303 |
| R9 | H2 + O2 → 2OH | 0.0303 |
| R10 | H2 + HO2 → 2OH + H | 0.0303 |
| R11 | O2 + OH → O + HO2 | 0.0227 |
| R12 | H + HO2 → H2O2 | 0.0227 |
| R13 | H2 + HO2 → OH + H2O | 0.0227 |
| R14 | OH → H + O | 0.0151 |
| R15 | H2 + O2 → O + H2O | 0.0151 |
| R16 | H2 + HO2 → H + H2O2 | 0.0151 |
| R17 | O + OH → HO2 | 0.0075 |
| R18 | O2 + OH → O2 + O + H | 0.0075 |
| R19 | HO2 + OH → 2O + H2O | 0.0075 |
| R20 | HO2 + H → 2OH | 0.0075 |
| R21 | H + HO2 → 2OH | 0.0075 |
| R22 | H2 + O → H + OH | 0.0075 |
| R23 | H2 + O2 → OH + H + O | 0.0075 |
| R24 | H2O2 → O + H2O | 0.0075 |
| R25 | H2 + O2 → H2O2 | 0.0075 |
| R26 | H2 + H2O2 → OH + H + H2O | 0.0075 |
| R27 | 2OH → H2O2 | 0.0075 |
| R28 | 2H → H2 | 0.0075 |

# SI6. TIME DEPENDENCE OF HYDROGEN AND OXYGEN SEQUENCES

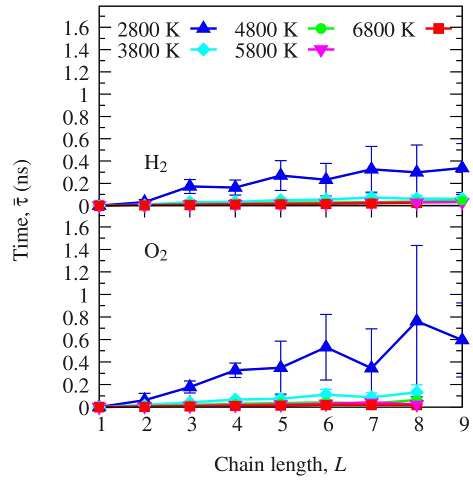


Figure 8: Average time, $\overline{\tau}$, to complete a sequence for hydrogen (top) and oxygen (bottom) at a range of temperature from 2800 to 6800 K and 250 $\mathrm{kg\,m^{-3}}$.

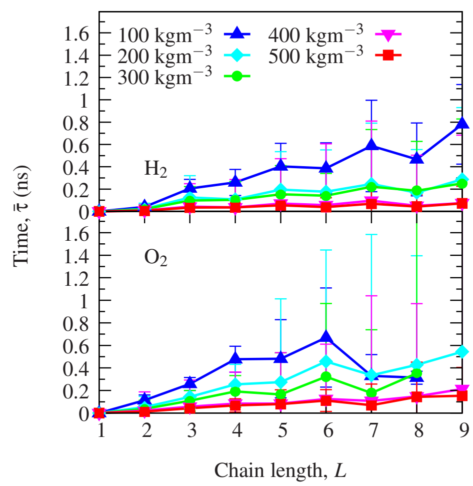


Figure 9: Average time, $\overline{\tau}$, to complete a sequence for hydrogen (top) and oxygen (bottom) at 3000 K and densities from 50 to 500 $\mathrm{kg\,m^{-3}}$.