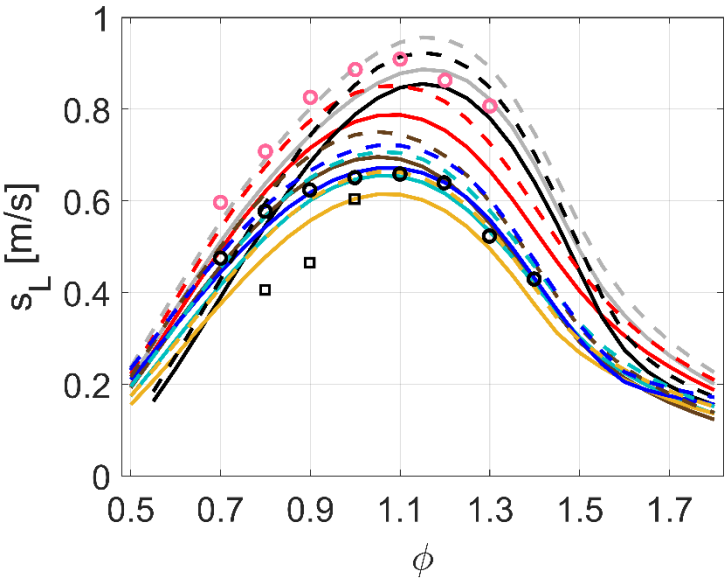
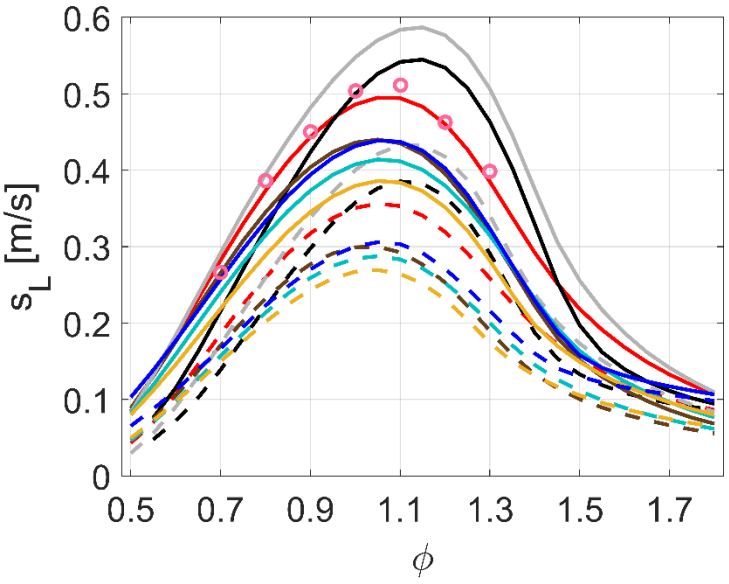
Supplementary Material

The relative relationships between the mechanisms are similar for both increasing gas temperatures, Fig. 1(a), as well as pressures, Fig. 1(b) as it is for the standard condition of 1 atm and 400 K (see figure in main article).

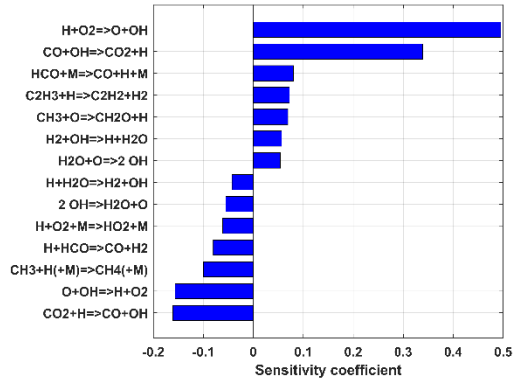


(a)

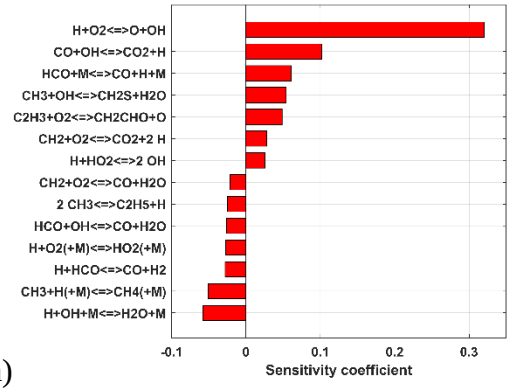


(b)

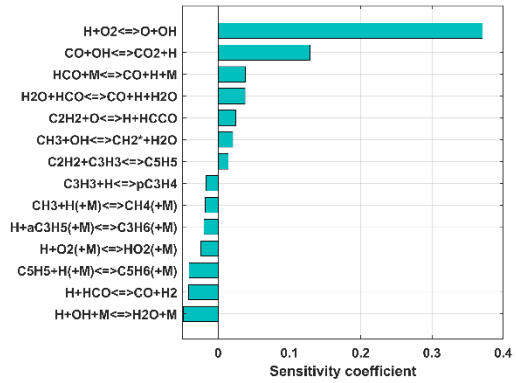
Fig. 1. Laminar burning velocities at (a) 1 atm and temperatures of 450 K (dashed) and 470 (solid) K, and (b) at 400 K and pressures of 3 (solid) and 10 (dashed) atm. Experimental laminar burning velocities for 1 atm and 450 K; JP-10: (□) [Parsinejad2006]. Limonene ($C_{10}H_{16}$): (○) [Courty2012]. For 1 atm and 470 K; N-$C_{10}H_{22}$: (○) [Kumar2007_CF]. For 3 atm and 400 K; N-$C_{10}H_{22}$: (○) [Hui2013]. Modelling; Z77 (blue), R5591 (red), T841 (lavender), T232 (yellow), C5-843 *(brown), SD206 (grey) and C184 (black).*


H+O2=>O+OH
CO+OH=>CO2+H
HCO+M=>CO+H+M
C2H3+H=>C2H2+H2
CH3+O=>CH2O+H
H2+OH=>H+H2O
H2O+O=>2 OH
H+H2O=>H2+OH
2 OH=>H2O+O
H+O2+M=>HO2+M
H+HCO=>CO+H2
CH3+H(+M)=>CH4(+M)
O+OH=>H+O2
CO2+H=>CO+OH
-0.2 -0.1 0 0.1 0.2 0.3 0.4 0.5
Sensitivity coefficient

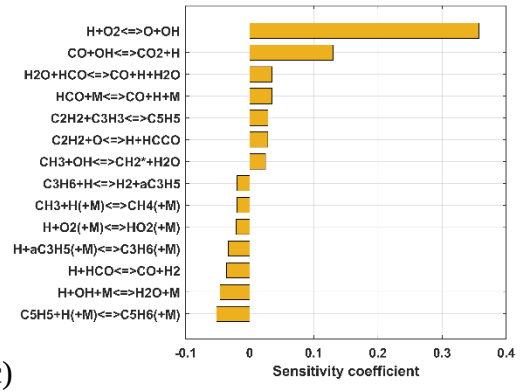
(a)


H+O2<=>O+OH
CO+OH<=>CO2+H
HCO+M<=>CO+H+M
CH3+OH<=>CH2S+H2O
C2H3+O2<=>CH2CHO+O
CH2+O2<=>CO2+2 H
H+HO2<=>2 OH
CH2+O2<=>CO+H2O
2 CH3<=>C2H5+H
HCO+OH<=>CO+H2O
H+O2(+M)<=>HO2(+M)
H+HCO<=>CO+H2
CH3+H(+M)<=>CH4(+M)
H+OH+M<=>H2O+M
-0.1 0 0.1 0.2 0.3
Sensitivity coefficient

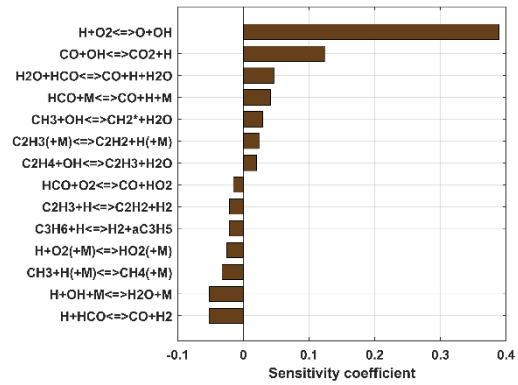
(b)


H+O2<=>O+OH
CO+OH<=>CO2+H
HCO+M<=>CO+H+M
H2O+HCO<=>CO+H+H2O
C2H2+O<=>H+HCCO
CH3+OH<=>CH2*+H2O
C2H2+C3H3<=>C5H5
C3H3+H<=>pC3H4
CH3+H(+M)<=>CH4(+M)
H+aC3H5(+M)<=>C3H6(+M)
H+O2(+M)<=>HO2(+M)
C5H5+H(+M)<=>C5H6(+M)
H+HCO<=>CO+H2
H+OH+M<=>H2O+M
0 0.1 0.2 0.3 0.4
Sensitivity coefficient

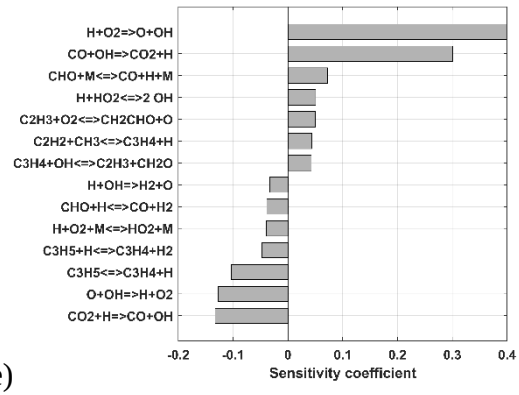
(c)


H+O2<=>O+OH
CO+OH<=>CO2+H
H2O+HCO<=>CO+H+H2O
HCO+M<=>CO+H+M
C2H2+C3H3<=>C5H5
C2H2+O<=>H+HCCO
CH3+OH<=>CH2*+H2O
C3H6+H<=>H2+aC3H5
CH3+H(+M)<=>CH4(+M)
H+O2(+M)<=>HO2(+M)
H+aC3H5(+M)<=>C3H6(+M)
H+HCO<=>CO+H2
H+OH+M<=>H2O+M
C5H5+H(+M)<=>C5H6(+M)
-0.1 0 0.1 0.2 0.3 0.4
Sensitivity coefficient

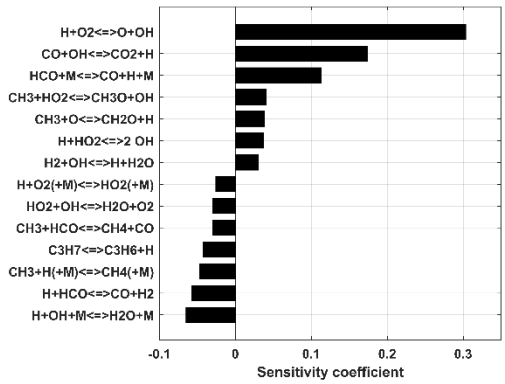
(d)


H+O2<=>O+OH
CO+OH<=>CO2+H
H2O+HCO<=>CO+H+H2O
HCO+M<=>CO+H+M
CH3+OH<=>CH2*+H2O
C2H3(+M)<=>C2H2+H(+M)
C2H4+OH<=>C2H3+H2O
HCO+O2<=>CO+HO2
C2H3+H<=>C2H2+H2
C3H6+H<=>H2+aC3H5
H+O2(+M)<=>HO2(+M)
CH3+H(+M)<=>CH4(+M)
H+OH+M<=>H2O+M
H+HCO<=>CO+H2
-0.1 0 0.1 0.2 0.3 0.4
Sensitivity coefficient

(e)


H+O2=>O+OH
CO+OH=>CO2+H
CHO+M<=>CO+H+M
H+HO2<=>2 OH
C2H3+O2<=>CH2CHO+O
C2H2+CH3<=>C3H4+H
C3H4+OH<=>C2H3+CH2O
H+OH=>H2+O
CHO+H<=>CO+H2
H+O2+M<=>HO2+M
C3H5+H<=>C3H4+H2
C3H5<=>C3H4+H
O+OH=>H+O2
CO2+H=>CO+OH
-0.2 -0.1 0 0.1 0.2 0.3 0.4
Sensitivity coefficient

(f)


H+O2<=>O+OH
CO+OH<=>CO2+H
HCO+M<=>CO+H+M
CH3+HO2<=>CH3O+OH
CH3+O<=>CH2O+H
H+HO2<=>2 OH
H2+OH<=>H+H2O
H+O2(+M)<=>HO2(+M)
HO2+OH<=>H2O+O2
CH3+HCO<=>CH4+CO
C3H7<=>C3H6+H
CH3+H(+M)<=>CH4(+M)
H+HCO<=>CO+H2
H+OH+M<=>H2O+M
-0.1 0 0.1 0.2 0.3
Sensitivity coefficient

(g)

Fig. 2. Sensitivity analysis of the 14 most important reactions for laminar burning velocities, at 1 atm, 400 K and φ=1.0. Z77 in blue (a), R5591 in red (b), T841 in lavender (c), T232 in yellow (d), C5-843 in brown (e), SD206 in grey (e) and C184 in black (g).

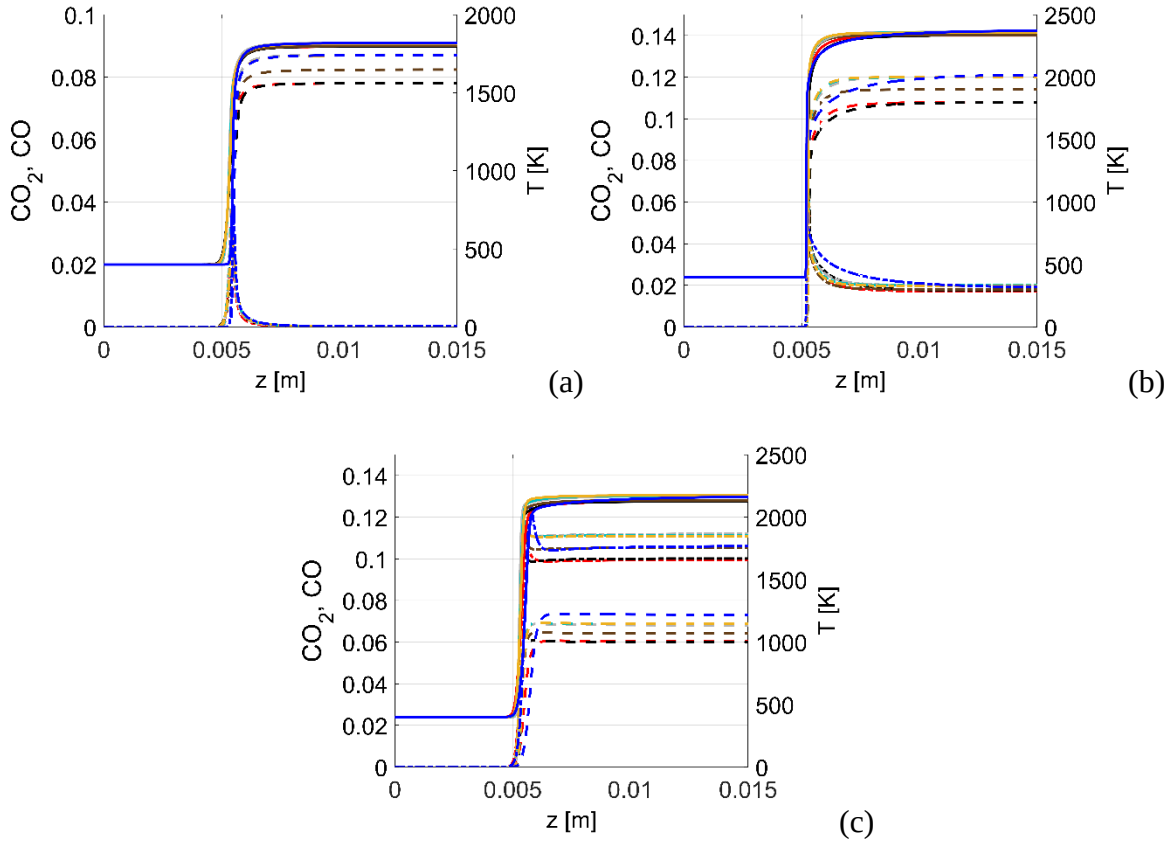


Fig. 3. Flame profiles of molar concentrations of CO_2 (dashed) and CO (dot-dashed) on the left axis and temperature (solid) on the right axis, at initial conditions of 1 atm and 400 K, and equivalence ratios of φ=0.6 in (a), φ=1.0 in (b) and φ=1.4 in (c). Z77 (blue), R5591 (red), T841 (lavender), T232 (yellow), C5-843 *(brown), SD206 (grey) and C184 (black).*

[Parsinejad2006] Parsinejad, F., Arcari, C., & Metghalchi, H. (2006). Flame structure and burning speed of JP-10 air mixtures. *Combustion science and technology*, *178*(5), 975-1000.

[Court2012] Courty, L., Chetehouna, K., Halter, F., Foucher, F., Garo, J. P., & Mounaïm-Rousselle, C. (2012). Experimental determination of emission and laminar burning speeds of α-pinene. *Combustion and flame*, *159*(4), 1385-1392.

[Kumar2007_CF] Kumar, K., & Sung, C. J. (2007). Laminar flame speeds and extinction limits of preheated n-decane/O2/N2 and n-dodecane/O2/N2 mixtures. *Combustion and Flame*, *151*(1-2), 209-224.

[Hui2013] Hui, X., & Sung, C. J. (2013). Laminar flame speeds of transportation-relevant hydrocarbons and jet fuels at elevated temperatures and pressures. *Fuel*, *109*, 191-200.

1. Courty, L., Chetehouna, K., Halter, F., Foucher, F., Garo, J. P., & Mounaïm-Rousselle, C. Experimental determination of emission and laminar burning speeds of α-pinene. *Combust. Flame* **159**, 1385–1392 (2012).
2. H. Wang personal communication. *https://web.stanford.edu/group/haiwanglab/HyChem/pages/download.html* (20200420).
3. Parsinejad, F., Arcari, C., & Metghalchi, H. Flame structure and burning speed of JP-10 air mixtures. *Combust. Sci. Technol.* **178**, 975–1000 (2006).