Application of the Fernandez-Terrazo et al. one-step chemistry model for partially premixed combustion to n-heptane.

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A set of model parameters has been derived for the use of the model with n-heptane following the procedure set out by Fernandez et al.

q equals 4501kJ/mol for n-heptane combustion, and we use the suggested expression for q as a function of equivalence ratio:

$\phi \le 1 : q / q_0 = 1,$

$\phi \ge 1 : q / q_0 = 1 - \alpha(\phi - 1),$

A suggested value of alpha for n-heptane is 0.18. The resulting adiabatic flame temperatures are shown in figure 1.

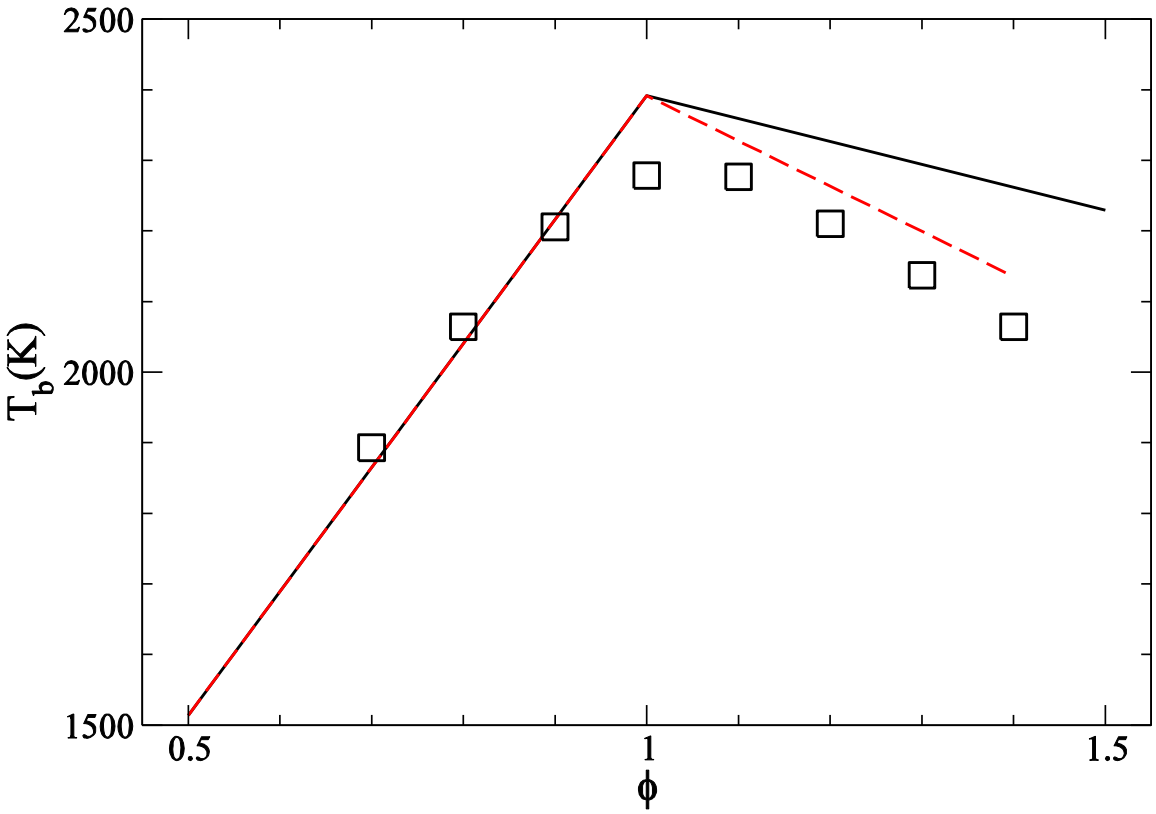


Fig 1. Solid line :q=qo; Dashed line q=q(phi); Symbols are equilibrium calculations by Huang.

The activation energy is estimated using

$$T_a = \frac{\alpha T_b^2 (T^0 - T^u)}{(T_b - T^0)(T_b - T_u)}$$

The value of alpha from theory equals 2.0, however Muller gives an empirical value of 2.3 for n-heptane. The inner layer temperature T^0 is given as 1244 to 1288 K depending on phi. This results in a range of values for Ta is 10500K (phi=1 and n=2) to 18000K (phi =0.7 and n=2.3) which may be appropriate. Plotting the laminar flame speed (using COSILAB with detailed transport) for values of Ta between 10000K and 160000 suggested that Ta=15000K, B=2.4 x 10^14(cm^3/mol s) was a reasonable value to use, however the values from 13000 to 16000K were within the range of experimental results.

The flame speeds were then recalculated using variable heat of reaction defined above. Finally the exact activation temperature needed to obtain the flame speeds given by Davis were obtained for rich mixture fractions, and a second order polynomial was fitted through the available values. While a constant activation temperature gives a good fit to the date on the lean side a quadratic variation with phi was also used there to ensure that reaction rates fall off quickly outside the flammable range (approx. phi =0.5 to phi=3.5). The resulting flame speeds are compared with experimental data in figure 2

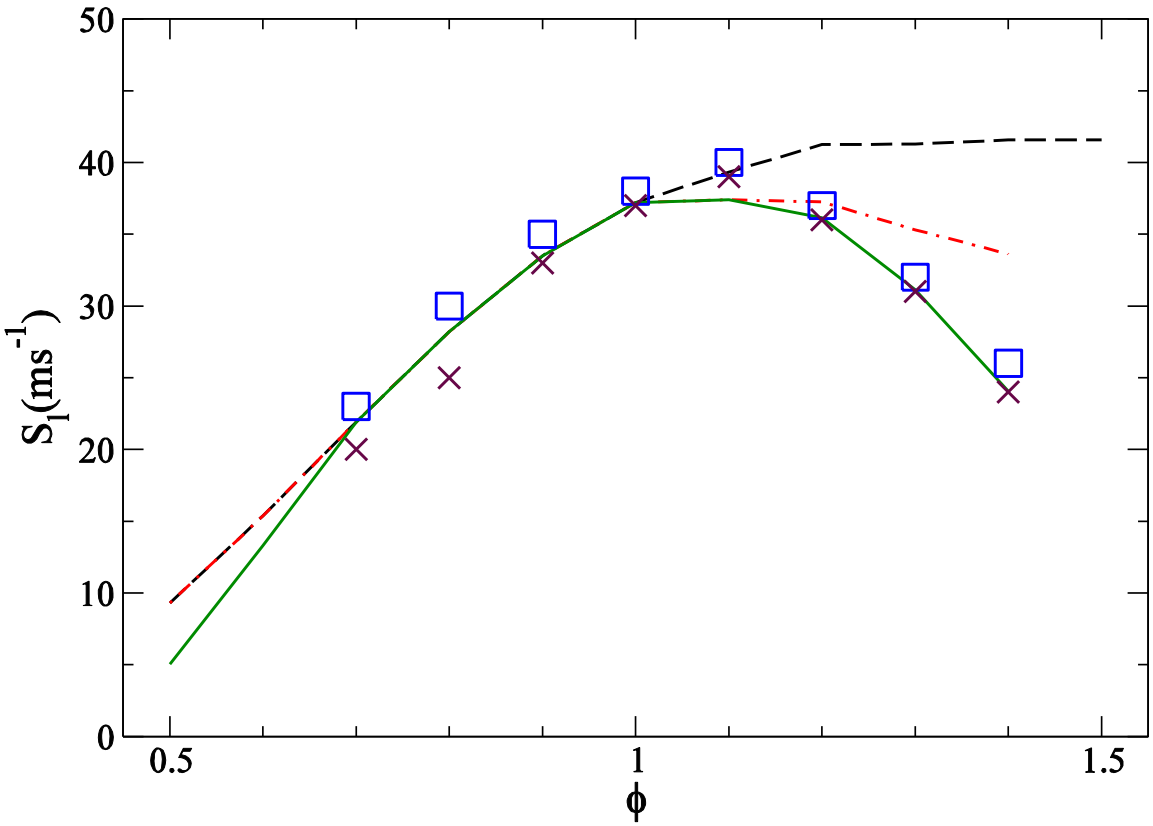


Fig. 2. Dashed line: constant q and Ta; Dot - dashed line: constant Ta; Solid line: Full model; Squares: measurements by Huang et al.; Crosses: measurements by Davis et al.

The resulting model is as given in the Fernandez-Terrazo et al. paper with the activation temperature given by:

$\phi \le 0.74$:

$Ta/Tao = 1 + 1.6948(\phi - 0.74)^2$

$1.13 \ge \phi \ge 0.74$:

$Ta/Tao = 1$

$\phi \ge 1.13$:

$Ta/Tao = 1 + 0.0092(\phi - 1) + 0.9423(\phi - 1.13)^2$

The resulting model is seen to give reasonable predictions in a non-premixed 0D Conditional Moment Closure calculation. The variation of the maximum temperature with peak scalar dissipation rate (amplitude mapping closure) is shown in figure 3, and the conditional profiles are shown immediately prior to ignition (N_ext=190 (1/s)) showing significant fuel leakage through the flame. These will need to be checked against a more detailed mechanism. From my own experience I guess the extinction value is not out by more than a factor of two.

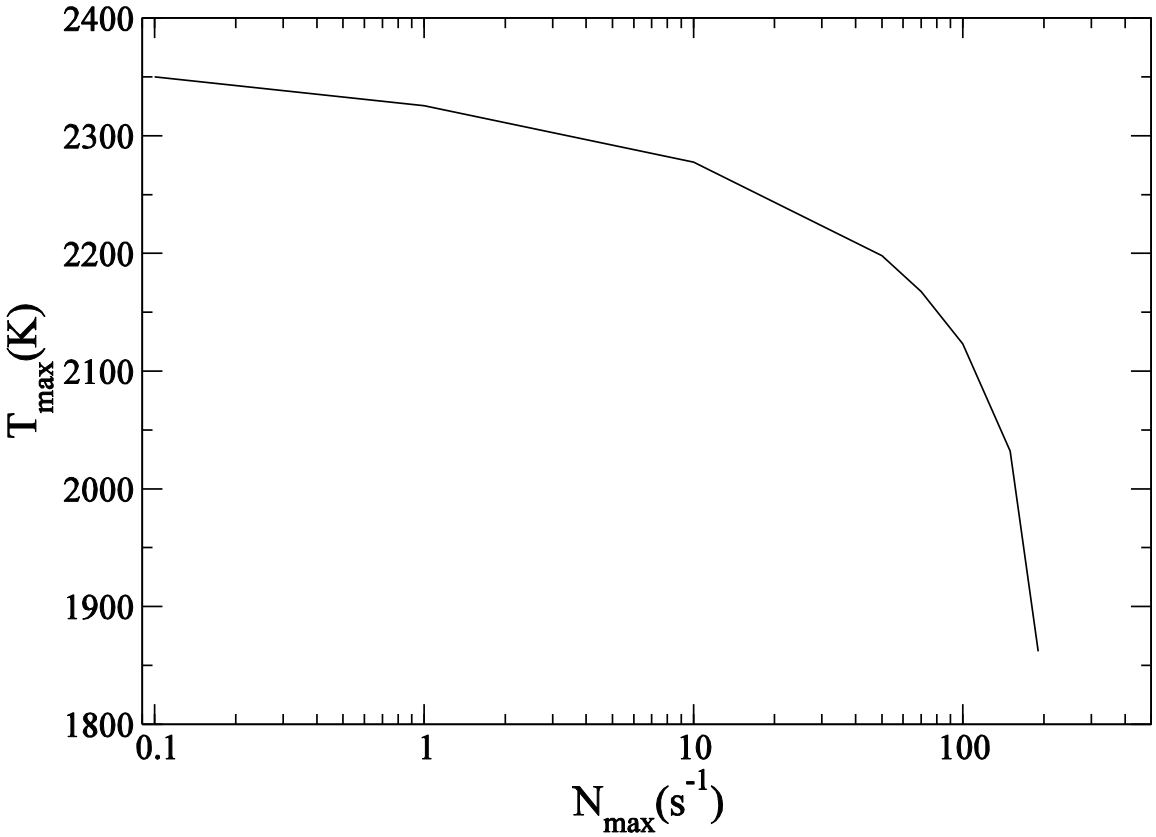
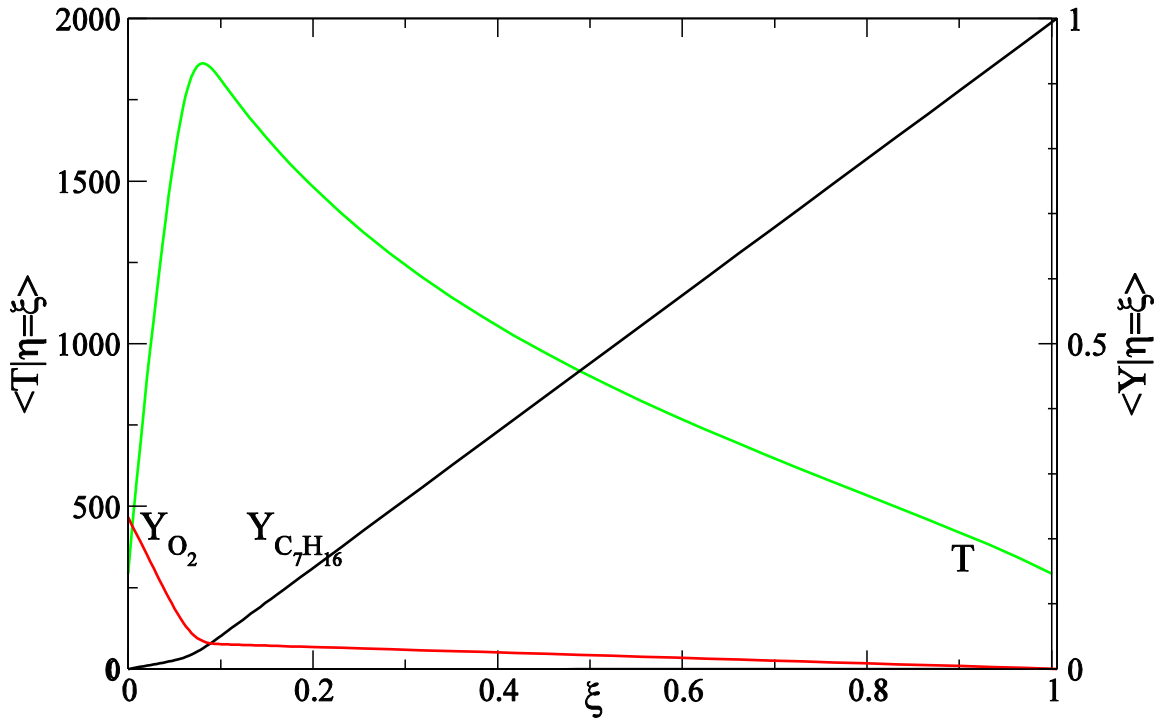


Fig. 3, Tmax versus peak scalar dissipation rate for 0D CMC, with the AMC model.



Conditional reactant and temperature profiles in mixture fraction at 99.5% of the extinction strain rate.

References:

Huang et al. Combust. Flame 139:239-251(2004)
Muller et al. Combust. Flame 108:349-356(1997)
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