Supplementary Material of: Assessment of Approximate Soret Diffusion Models for Hydrogen and Ammonia Combustion

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A: Soret diffusion coefficients of heavy species

Figure 1 shows the Soret diffusion coefficient through an atmospheric $C_{10}H_{20}$ 1D freely propagating flame at stoichiometric condition, computed with the reaction mechanism by Franzelli et al. [1]. For larger species like this, the C&C model (orange dotted line) provides very good agreement with the reference values from the multicomponent model (black solid line), while the Bartlett model performs reasonably well. Note that the H&W model was derived assuming light species.

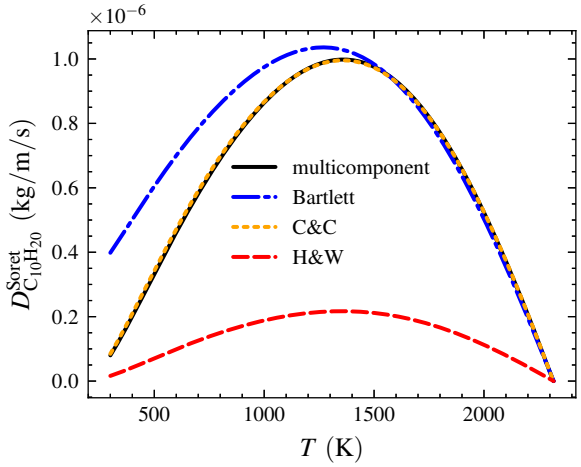

Fig. 1: Soret diffusion coefficient for $C_{10}H_{20}$ along a 1D freely propagating kerosene-air flame at atmospheric conditions and $\phi = 1$.

B: Laminar flame speeds from different hydrogen mechanisms

Comparison of laminar flame speeds from two reaction mechanism (Burke et al. [2] and Boivin [3]) in addition to the results from the Li et al. [4] mechanism in the main manuscript.

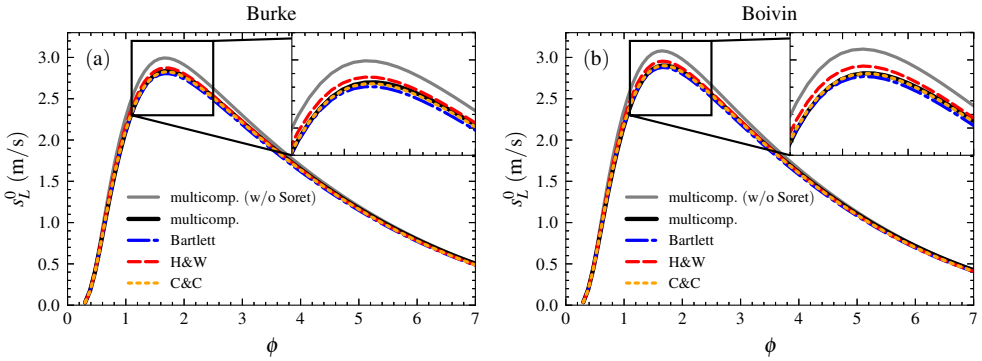

Fig. 2: Laminar flame speed s_L^0 for hydrogen-air flames at atmospheric conditions from the reaction mechanisms by (a) Burke et al. [2] and (b) Boivin [3]. The subplots in the top right corners show a zoom to the near-stoichiometric region where absolute differences between models are largest.

C: Comparison of flame speeds with measurements

The flame speeds from the different models presented in the main manuscript are laid on top of experimental measurements in Fig. 3 collected in a recent review paper by Han et al. [5]. The difference between all models lies well within the spread of the experimental data.

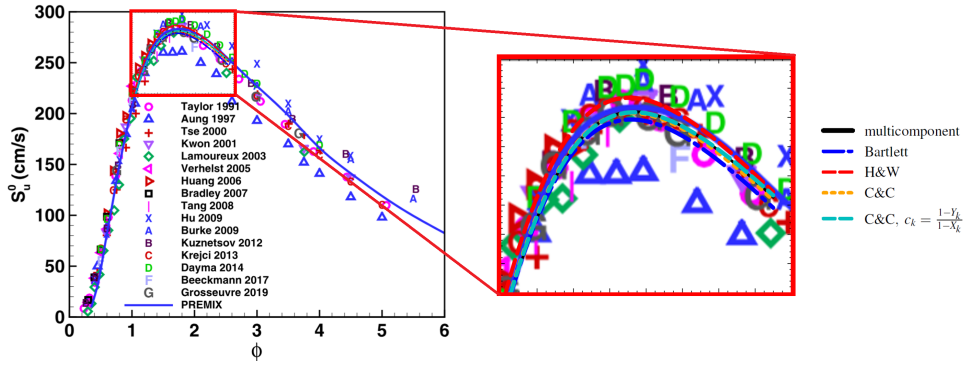

Fig. 3: Presented flame speeds from the main manuscript overlaid on top of collected experimental data from a recent review paper by Han et al. [5]

D: Premixed counterflow flames for ammonia/hydrogen blends with different reaction mechanisms

To make sure that the results shown for the ammonia/hydrogen counterflow flames from the main manuscript are independent of the choice of reaction mechanism, we repeated the simulations of the premixed counterflow flame for the 60/40 ammonia/hydrogen fuel blend with the KAUST mechanism [6] and the mechanism by Konnov [7]. While the KAUST mechanism yields results similar to the one by Stagni et al. (see Fig. 4), flame dynamics differ when using the mechanism by Konnov (Fig. 5). Nonetheless, the same trends in terms of Soret model accuracy found for the Stagni mechanism also hold for these two mechanisms.

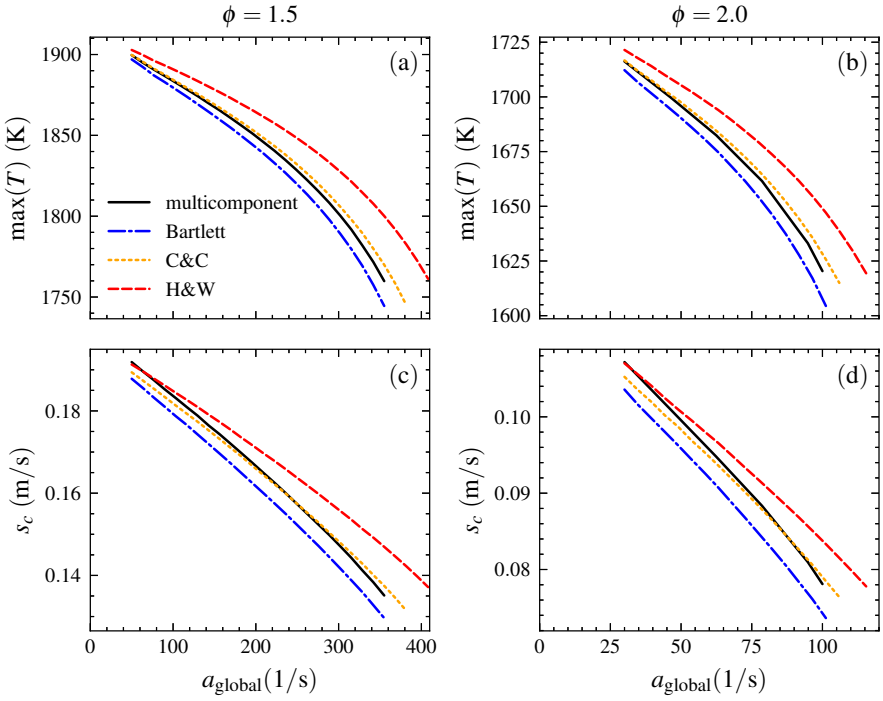

Fig. 4: Maximum temperature (top) and consumption speed (bottom) of rich ammonia/hydrogen flames (60 vol-% ammonia, 40 vol-% hydrogen) at two equivalence ratios (left and right) plotted as a function of flame stretch. Simulations performed with the KAUST mechanism [6].

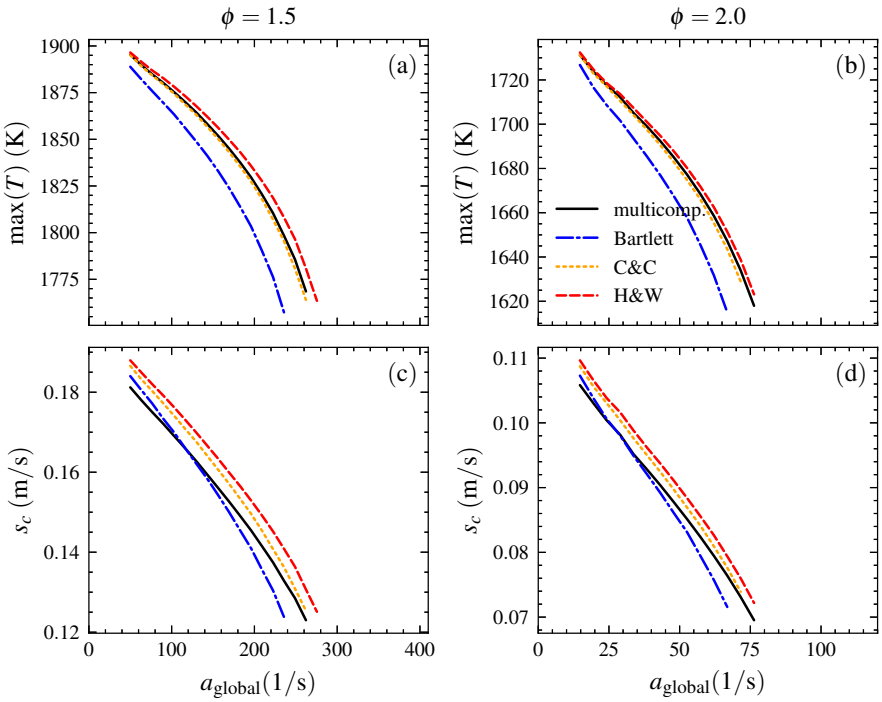

Fig. 5: Maximum temperature (top) and consumption speed (bottom) of rich ammonia/hydrogen flames (60 vol-% ammonia, 40 vol-% hydrogen) at two equivalence ratios (left and right) plotted as a function of flame stretch. Simulations performed with the Konnov mechanism [7].

E: Non-premixed ammonia/hydrogen counterflow flame

Generally, Soret diffusion is expected to play a larger role in premixed compared to non-premixed combustion. Figure 6 shows a non-premixed ammonia-air flame (60 vol-% ammonia, 40 vol-% hydrogen, atmospheric conditions) at $a_{\mathrm{global}} = 700\,1/\mathrm{s}$ computed with the Stagni mechanism. While main species profiles agree generally well, minor deviations are found for the hydrogen radical. A more in-depth study of non-premixed flames is beyond the scope of this work.

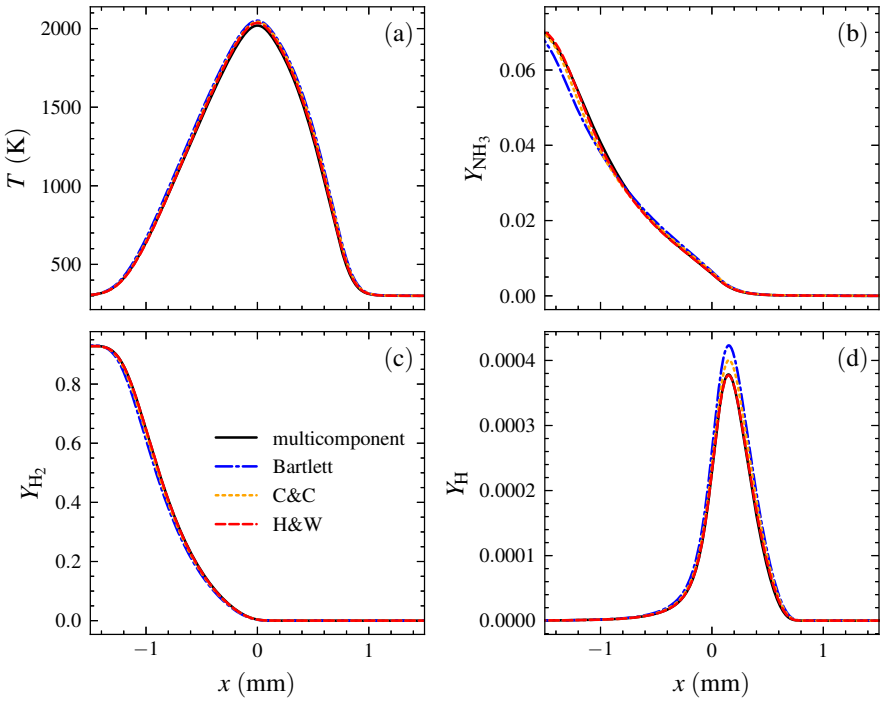

Fig. 6: Ammonia/hydrogen (60/40) non-premixed counterflow flame at $a_{\mathrm{global}} = 700\,\mathrm{s}^{-1}$. Presented are profiles of temperature (a), ammonia mass fraction (b), molecular hydrogen (c) and atomic hydrogen (d). $x = 0$ is the point of maximum temperature.

References

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