



Figure S4 Comparison of the measured laminar burning velocities of *n*-hexane/air mixtures at 1-10 atm and 353 K by Kelley et al. ^[9] (symbols) and simulated results of the present model (lines).

References

1. Peukert SL, Sivaramakrishnan R, Michael JV. 2015. High temperature rate constants for H/D+n-C₄H₁₀ and i-C₄H₁₀. *Proceedings of the Combustion Institute* 35:171-79
2. Orme JP, Curran HJ, Simmie JM. 2006. Experimental and modeling study of methyl cyclohexane pyrolysis and oxidation. *The Journal of Physical Chemistry A* 110:114-31
3. Badra J, Elwardany A, Farooq A. 2015. Shock tube measurements of the rate constants for seven large alkanes + OH. *Proceedings of the Combustion Institute* 35:189-96
4. Goos E, Hippler H, Hoyer mann K, Jürges B. 2001. Reactions of methyl radicals with isobutane at temperatures between 800 and 950 Kelvin. *International Journal of Chemical Kinetics* 33:732-40
5. Zhukov VP, Sechenov VA, Starikovskii AY. 2004. Ignition delay times in lean n-hexane-air mixture at high pressures. *Combustion and Flame* 136:257-59
6. Zhang KW, Banyon C, Burke U, Kukkadapu G, Wagnon SW, et al. 2019. An experimental and kinetic modeling study of the oxidation of hexane isomers: Developing consistent reaction rate rules for alkanes. *Combustion and Flame* 206:123-37
7. Ji C, Dames E, Wang YL, Wang H, Egolfopoulos FN. 2010. Propagation and extinction of premixed C₅-C₁₂ n-alkane flames. *Combustion and Flame* 157:277-87
8. Li X, Hu E, Lu X, Huang S, Huang Z. 2019. Experimental and kinetic study on laminar flame speeds of hexene isomers and n-hexane. *Fuel* 243:533-40
9. Kelley AP, Smallbone AJ, Zhu DL, Law CK. 2011. Laminar flame speeds of C₅ to C₈ n-alkanes at elevated pressures: Experimental determination, fuel similarity, and stretch sensitivity. *Proceedings of the Combustion Institute* 33:963-70
10. Yasunaga K, Yamada H, Oshita H, Hattori K, Hidaka Y, Curran H. 2017. Pyrolysis of n-pentane, n-hexane and n-heptane in a single pulse shock tube. *Combustion and Flame* 185:335-45