

The figures in this appendix are included in the following work and are reproduced with permission:

Burke, S., Burke, U., Mathieu, O., Osorio, I., Keesee, C., Morones, A., Petersen, E. L., Wang, W., DeVerter, T., Oehlschlaeger, M. A., Rhodes, B., Hanson, R. K., Davidson, D. F., Weber, B. W., Sung, C.-J., Santner, J., Ju, Y., Haas, F. M., Dryer, F. L., Volkov, E., Nilsson, E., Konnov, A., Alrefae, M., Khaled, F., Farooq, A., Dirrenberger, P., Glaude, P.-A., and Battin-Leclerc, F. “An Experimental and Modeling Study of Propene Oxidation. Part 2: Ignition Delay Time and Flame Speed Measurements.” *Combust. Flame*, (Submitted).

Propene is a foundational fuel that is an important step in the hierarchy of chemical kinetic models. Despite this, very few experiments have been conducted for propene at high-pressure, and low-to-intermediate temperature conditions. The data presented here substantially expand the available data sets for model validation.

In addition, this study was conducted in concert with collaborators at the National University of Ireland (NUI) at Galway, Texas A&M University, the King Abdullah University of Science and Technology, Stanford University, and Rensselaer Polytechnic Institute. The facilities utilized included two different RCMs and six different shock tubes; as such, this study represents one of the first comprehensive comparisons of homogeneous ignition in many experimental facilities.

That such a comparison is warranted is shown by Figs. 1 and 2. Figure 1 shows a comparison of the pressure traces from an experiment in the RCMs at UConn and NUI Galway. It is clear that, although the EOC pressures are similar, the pressure profiles pre- and post-EOC are quite different. The outcome of this difference in profile is evident in the difference in ignition delay displayed in Fig. 2. The ignition delays measured in the UConn RCM are shorter than those measured in the NUI Galway RCM in part because the pressure loss—and hence temperature loss—in the UConn RCM is less.

Figures 3–9 compare the results of the experiments in the various facilities to each other and to a model for propene developed in the work cited above. The symbols represent experimental data; simulations of the NUI Galway RCM and shock tube experiments are represented by solid lines;

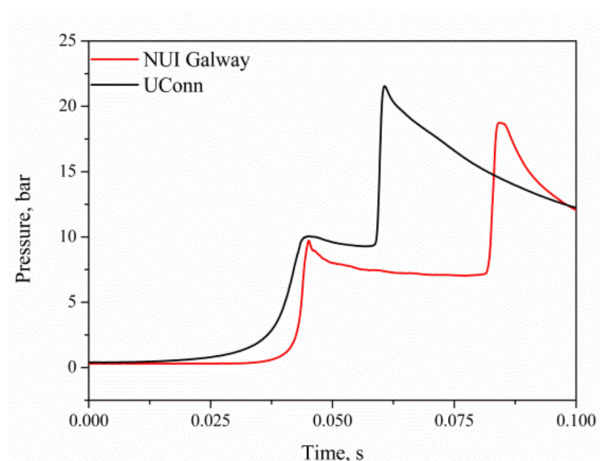


Figure 1: Comparison of pressure traces between the UConn and NUI Galway RCMs. $P_C = 10$ atm, $T_C \approx 1040$ K, $\phi = 1.0$, 12 %O₂.

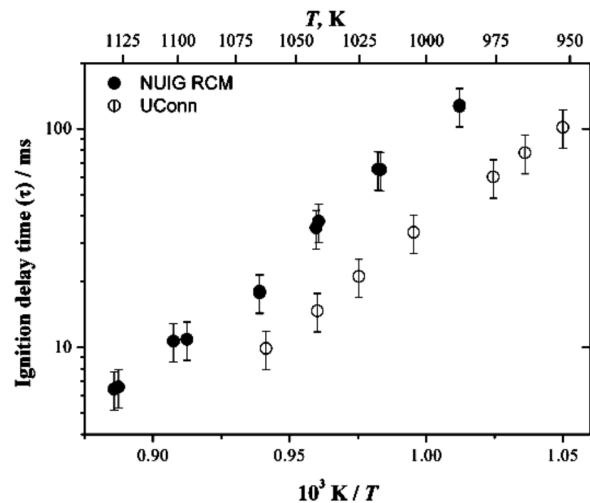


Figure 2: Comparison of ignition delays of propene measured in the UConn and NUI Galway RCMs. $P_C = 10$ atm, $\phi = 1.0$, 12 %O₂.

and simulations of the UConn RCM experiments are represented by dashed lines. In general, the agreement among the experiments and between the experiments and the model is quite good. Most importantly, the experiments are well modeled by the kinetic mechanism when the proper facility effects are applied to the simulation.

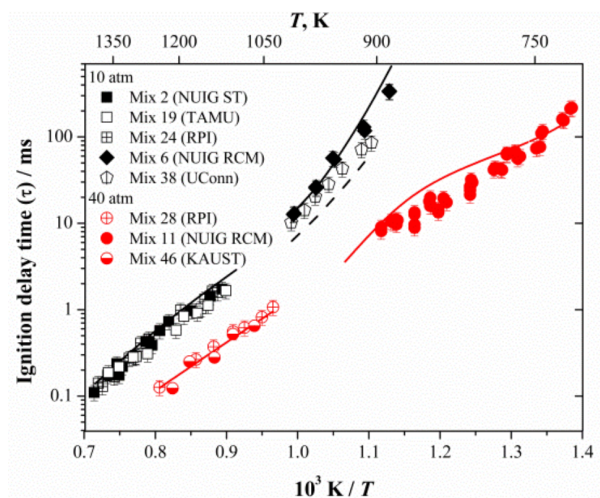


Figure 3: Ignition delays of propene in stoichiometric mixture with air at two pressures

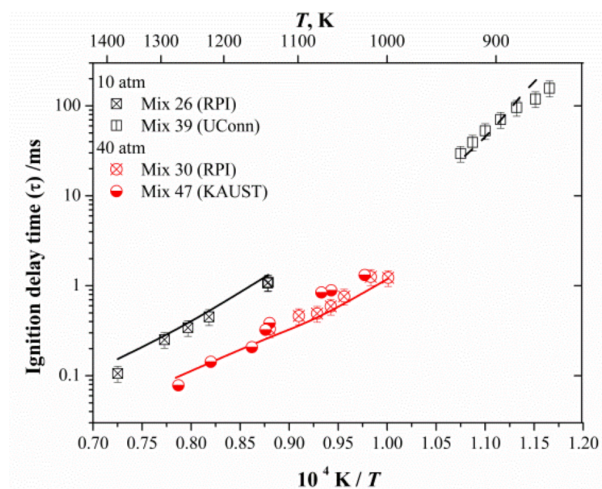


Figure 4: Ignition delays of propene in $\phi = 2.0$ mixture with air at two pressures

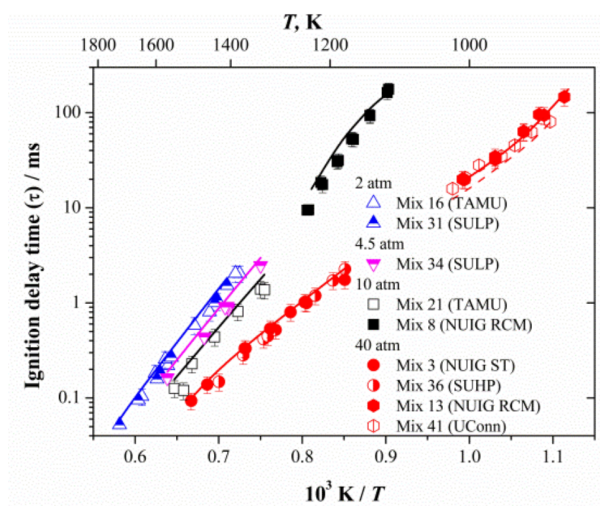


Figure 5: Ignition delays of propene with 4% O_2 , $\phi = 1.0$

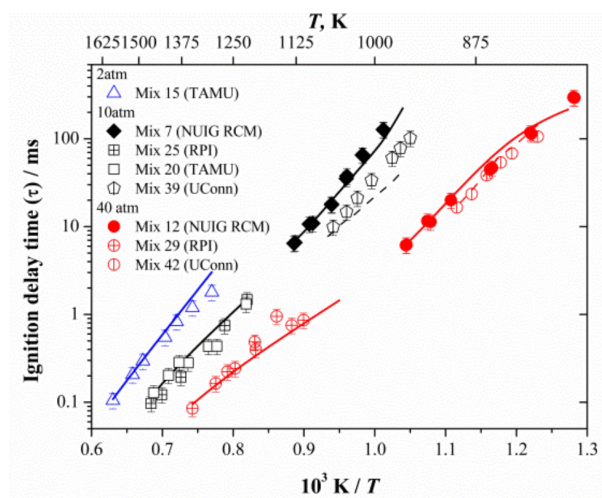


Figure 6: Ignition delays of propene with 12% O_2 , $\phi = 1.0$

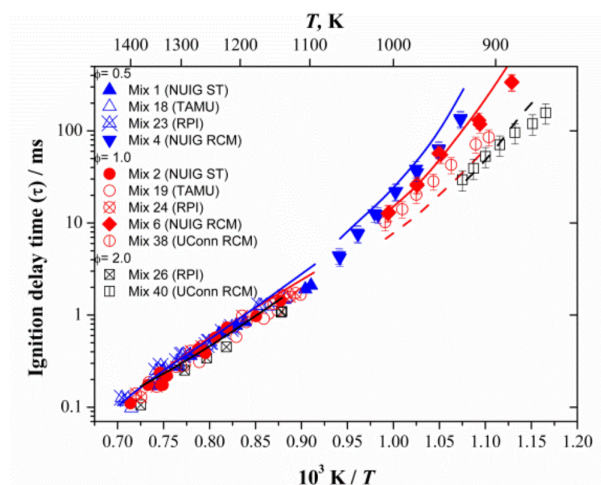


Figure 7: Ignition delays of propene with mixtures of air at 10 atm for three equivalence ratios

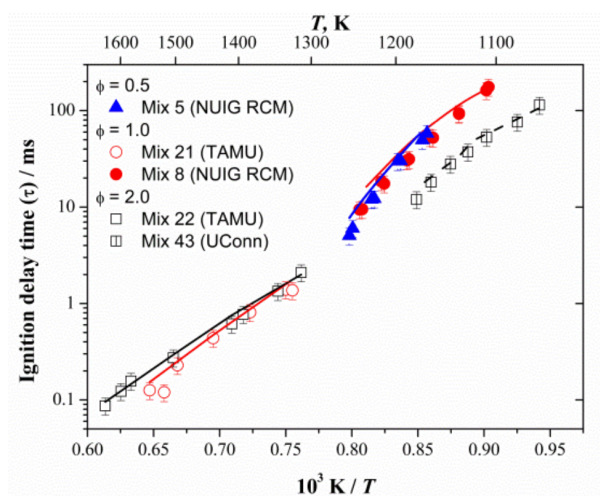


Figure 8: Ignition delays of propene with 4 % O_2 at 10 atm for three equivalence ratios

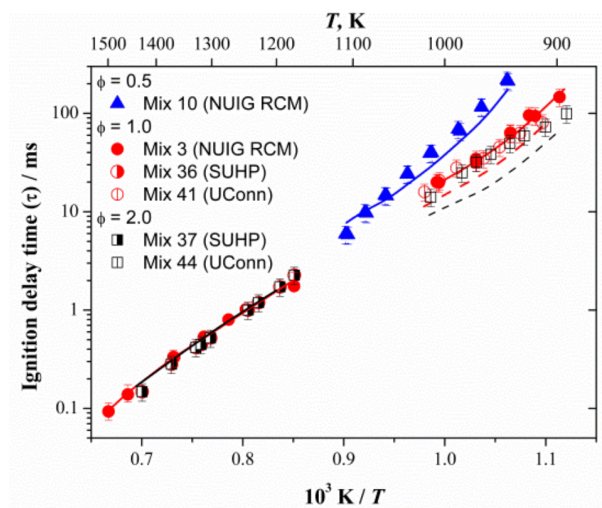


Figure 9: Ignition delays of propene with 4 % O_2 at 40 atm for three equivalence ratios