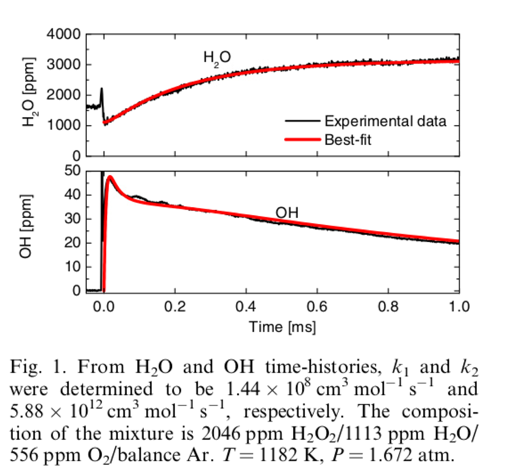
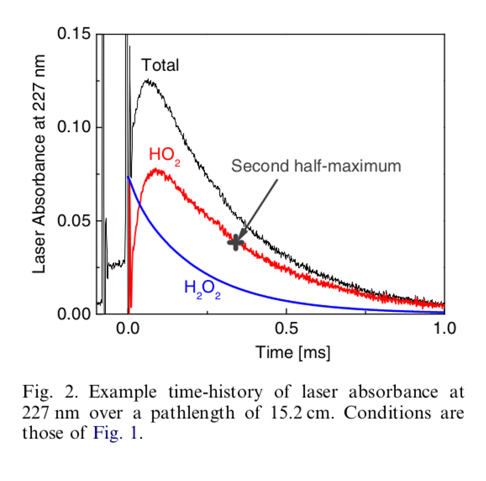
**Procedure to Recreate Data: Temperature Dependence for k1 and k2 and Constant values for k3 and k4**

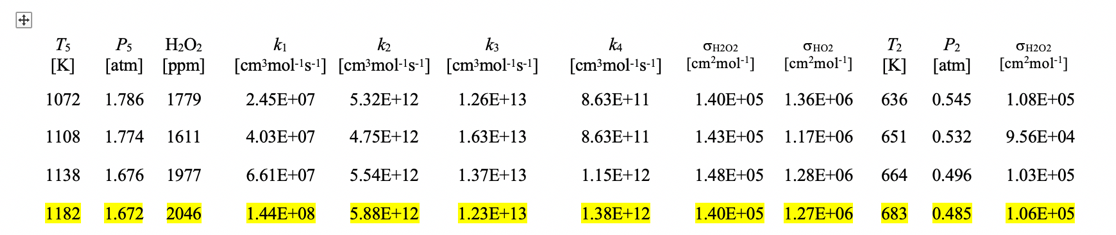
Procedure: The following procedure details how we attempted to recreate the raw data seen in the paper (Z. Hong, K. Lam, R. Sur, S. Wang, D. Davidson, R. Hanson, Proceedings of the Combustion Institute 34 (2013) 565-571.) In this approach we will use the two arrhenius expressions presented in the paper for k1 and k2 and the rate constant values presented in the supplemental material for k3 and k4.

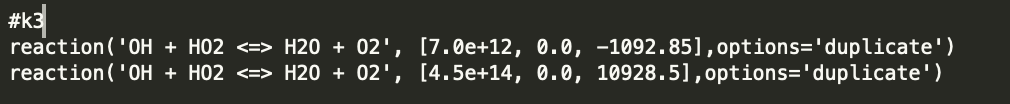
1. In order to obtain the raw data presented in the paper an online graph reader was used and the following three plots were graph-read to acquire data from the images presented in the paper
   1. Fig. 1 top (H2O ppm profile)
   2. Fig. 1 bottom (OH ppm profile)

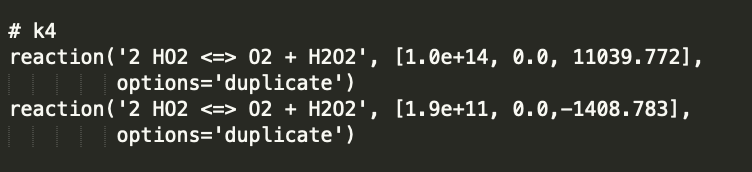


* 1. Fig. 2 Laser Absorbance

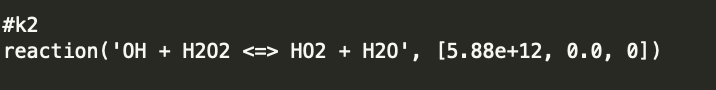
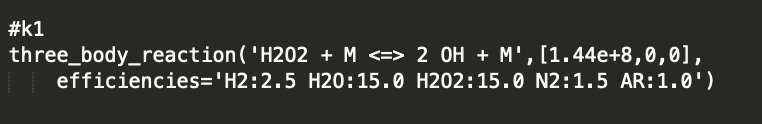


1. Downloaded the mechanism presented in the paper (Reference 14)
   1. Converted the mechanism file to a cti file in order to be able to run simulations using Cantera
2. Downloaded the supplementary material presented in the paper
   1. Located the conditions at which the raw data was determined
   2. 
3. Updated the key reactions in the cti file
   1. updated (k3,k4) with the expressions presented in the paper
      1. k3 = 7.0 X 1012exp(550/T) + 4.5 X 1014 exp(-5500/T)
      2. k4 = 1.0 X 1014exp(-5556/T) + 1.9 X 1011exp(709/T)





* 1. updated (k1,k2), with the values as seen above in the supplementary material
     1. This was done by setting the A factor for a given reaction equal to the rate constant, and setting other parameters equal to zero (for Example: A1 = k1, n1=0, Ea1=0).



1. Updated the absorption coefficients for H2O2 and HO2 internally in our code in order to match that of those in the supplementary material ()
2. Ran a constant pressure shock tube simulation using Cantera using the modified cti file and the pressure, temperature and initial mixture composition presented in the paper
   1. P = 1.672 atm
   2. T = 1182 K
   3. X =2046 ppm H2O2/1113 ppm H2O/556 ppm O2/balance Ar
3. Plotted the results

Plots Of The Results Can Be Seen Below:

Results for OH Profile



Results for H2O Profile



Results For Absorbance 227 nm Profile

