Dynamics of Excited Hydroxyl Radicals in Hydrogen Based Mixtures Behind Reflected Shock Waves

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Supplemental material

R. MÉVEL, S. PICHON, L. CATOIRE, N. CHAUMEIX, C.-E. PAILLARD and J.E. SHEPHERD

The present section provides some complementary results which were not included in the manuscript because of size restriction.

Results and discussion

Hydrogen peroxide-water vapour mixtures

Comparison of experimental and calculated profiles. Rate of production of OH and OH radicals.*

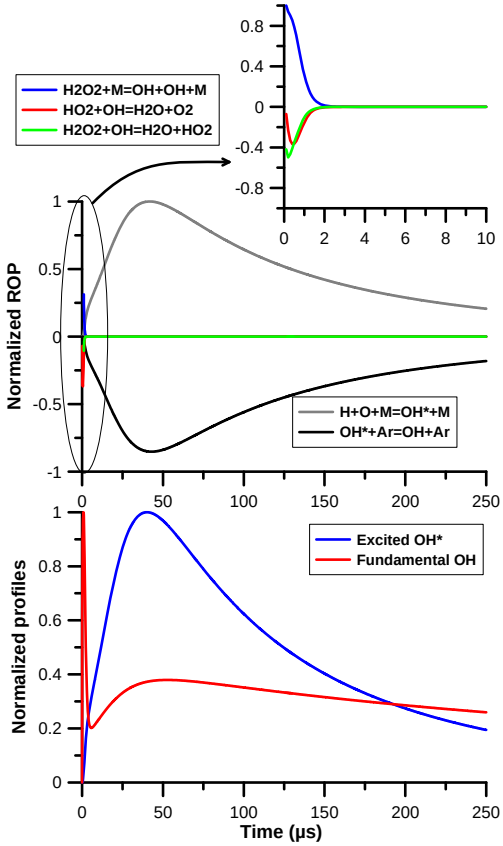

Figure S1: Rates of production, ROP, for OH* and OH (top) and experimental emission and calculated OH* and OH profiles (bottom) for a H_2-H_2O_2-H_2O-Ar mixture. Conditions: X_{H2}=0.01 ; X_{H2O2}=0.005527 ; X_{H2O}=0.004473 ; X_{Ar}=0.98 ; T_5=1450 K; P_5=300 kPa.

Temperature and temperature gradient profiles. Energy release rate per reaction analysis.

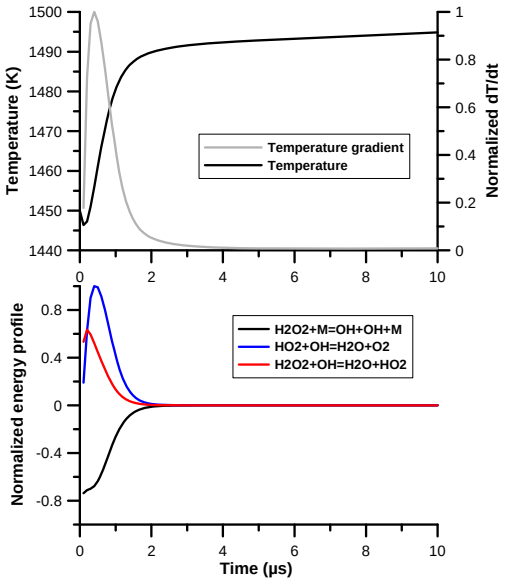

Figure S2: Calculated temperature and temperature gradient profile (top) and normalized energy release rates per reaction (bottom) for a H_2-H_2O_2-H_2O-Ar mixture. Conditions: X_{H2}=0.01 ; X_{H2O2}=0.005527 ; X_{H2O}=0.004473 ; X_{Ar}=0.98 ; T_5=1450 K; P_5=300 kPa.

Hydrogen-nitrous oxide(-oxygen) mixtures

Comparison of experimental and calculated profiles. Rate of production of OH and OH radicals.*

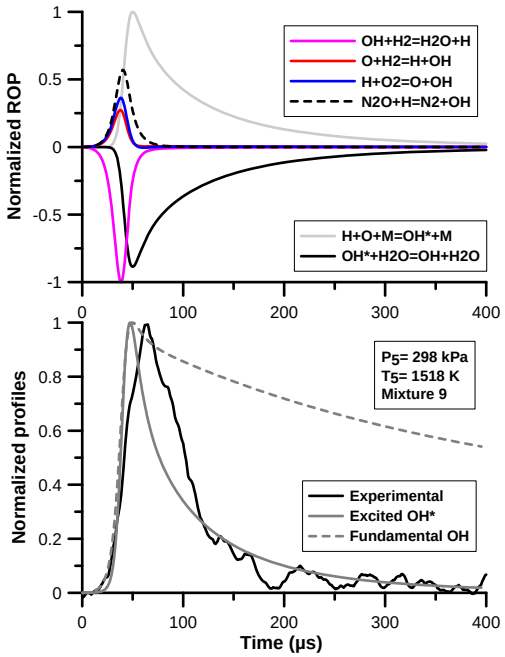

Figure S3: Rates of production, ROP, for OH* and OH (top) and experimental emission and calculated OH* and OH profiles (bottom) for a H_2-O_2-N_2O-Ar mixture.

Temperature and temperature gradient profiles. Energy release rate per reaction analysis.

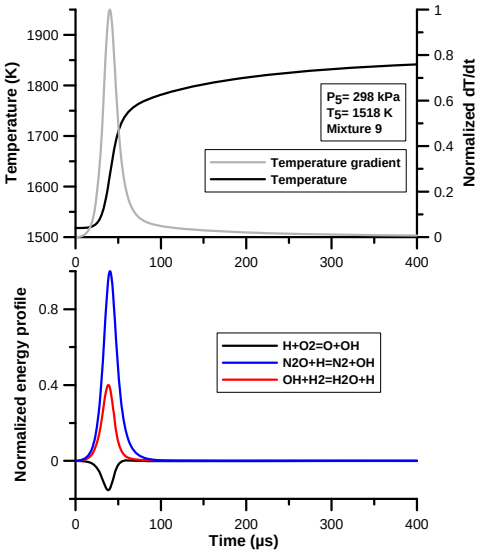

Figure S4: Calculated temperature and temperature gradient profile (top) and normalized energy release rates per reaction (bottom) for a H_2-O_2-N_2O-Ar mixture.

Comparison between $[OH^*]_{Full\_Model}$ and $[OH^*]_{Steady\_State}$

Hydrogen-oxygen mixtures

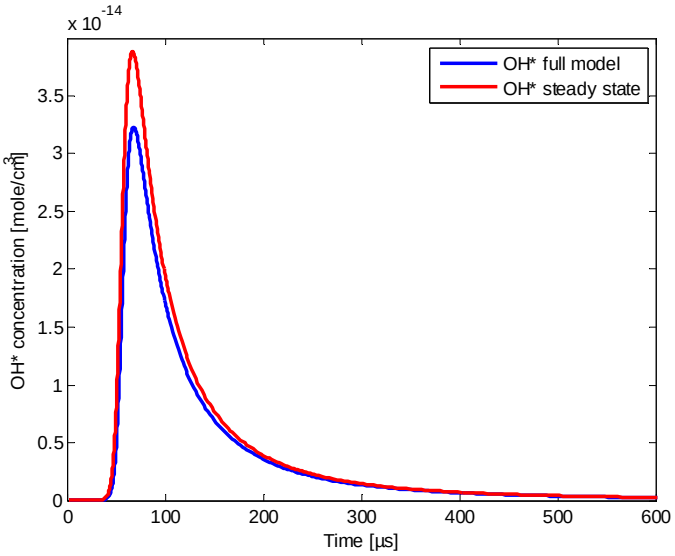

Figure S5: Comparison between the OH* concentrations obtained with the detailed reaction model and with the QSSA for a H_2-O_2-Ar mixture. Conditions: X_{H2}=0.02 ; X_{O2}=0.01 ; X_{Ar}=0.97 ; T=1450 K; P=303 kPa.

Hydrogen peroxide-water vapour mixtures

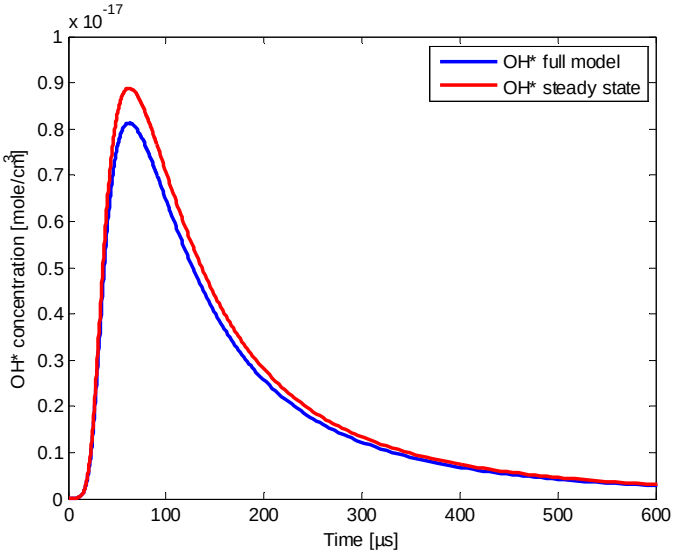

Figure S6: Comparison between the OH* concentrations obtained with the detailed reaction model and with the QSSA for a H_2O_2-H_2O-Ar mixture. Conditions: X_{H2O2}=0.0055 ; X_{H2O}=0.0045 ; X_{Ar}=0.99 ; T=1200 K; P=303 kPa.

Hydrogen-nitrous oxide mixtures

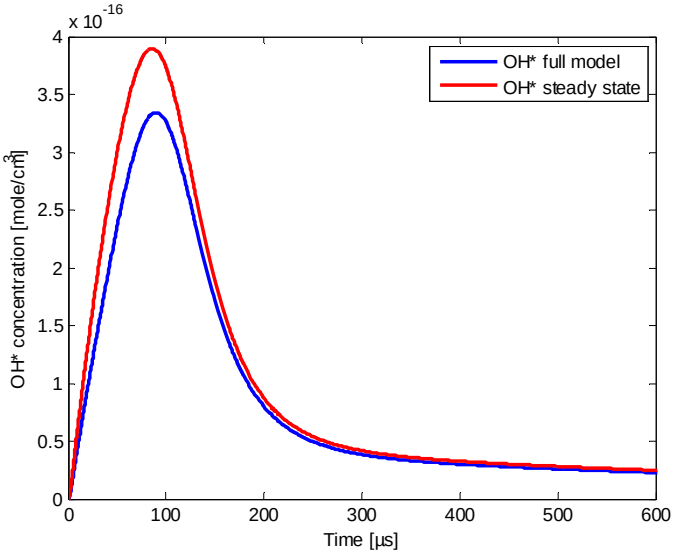

Figure S7: Comparison between the OH* concentrations obtained with the detailed reaction model and with the QSSA for a H_2-N_2O-Ar mixture. Conditions: X_{H2}=0.01; X_{N2O}=0.01; X_{Ar}=0.98; T=1650 K; P=303 kPa.

Hydrogen-nitrous oxide-oxygen mixtures

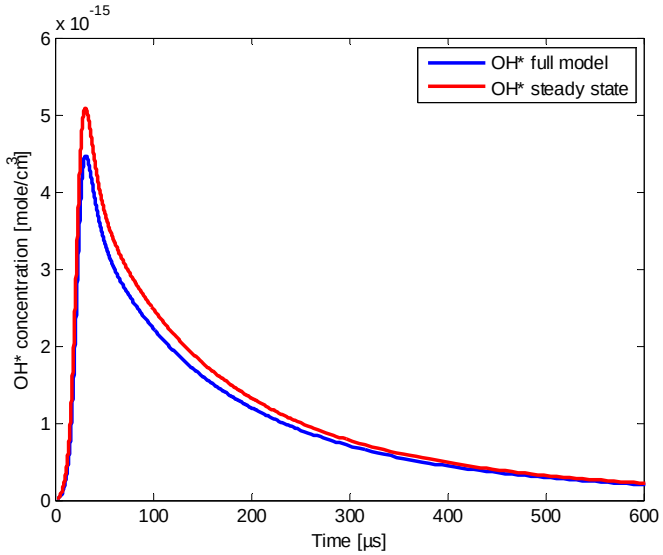

Figure S8: Comparison between the OH* concentrations obtained with the detailed reaction model and with the QSSA for a H_2-N_2O-O_2-Ar mixture. . Conditions: X_{H2}=0.01; X_{O2}=0.005; X_{N2O}=0.005; X_{Ar}=0.98; T=1800 K; P=303 kPa.

Comparison between several reaction models

List of reaction model tested

In each model, a sub-model for OH* chemistry was added for direct comparison with ignition delay time derived from emission at 306 nm.

Stanford:

Hong Z., Davidson D.F. and Hanson R.K., An improved H_2/O_2 mechanism based on recent shock tube/laser absorption measurements, Combustion and Flame 158 (2011) 633-644.

USC:

Wang H., Xiaoqing Y., Ameya V.J., Davis G.D., Laskin A., Egolfopoulos F. and Law C.K., USC Mech Version II. High-temperature combustion reaction model of $H_2/CO/C_1$-C_4 compounds. Available at: http://ignis.usc.edu/USC_Mech_II.htm, 2007.

GRI:

Smith G., Golden D., Frenklach M., Moriarty N., Eiteneer B., Goldenberg M., Bowman C., Hanson R., Song S., Gardiner W., Lissianski V., and Qin Z., GRI-mech release 3.0

Dagaut:

Le Cong T., Etude expérimentale et modélisation de la cinétique de combustion de combustibles gazeux : Méthane, gaz naturel et mélanges contenant de l'hydrogène, du monoxyde de carbone, du dioxyde de carbone et de l'eau, Université d'Orléans, 2007, 257 p.

Konnov:

Konnov A., Detailed reaction mechanism for small hydrocarbons combustion. Release 0.5., 2000.

Present study:

Mével R., Javoy S., Lafosse F., Chaumeix N., Dupré G., and Paillard C.-E., Hydrogen-nitrous oxide delay time: shock tube experimental study and kinetic modeling, Proceedings of The Combustion Institute, 2009, 32, 359-366.

Mével R., Javoy S., and Dupré G., A chemical kinetic study of the oxidation of silane by nitrous oxide, nitric oxide and oxygen, Proceedings of The Combustion Institute, 2011, 33, 485-492.

Pichon S., Etude cinétique de systèmes hypergoliques et propergoliques à base d'éthanol et de peroxide d'hydrogène, Université d'Orléans, 2005, 251 p.

Hydrogen peroxide-water vapor mixtures

Mixtures:
- N°6: X_{H2O2}=0.0055270; X_{H2O}=0.0044730; X_{Ar}=0.99.
- N°7: X_{H2O2}=0.0027635; X_{H2O}=0.0022365; X_{Ar}=0.995.

Delay-time definitions:
The delay-times are defined as the times to 50% and 100% of emission maximum.

Stanford model:

Mean error =59 %

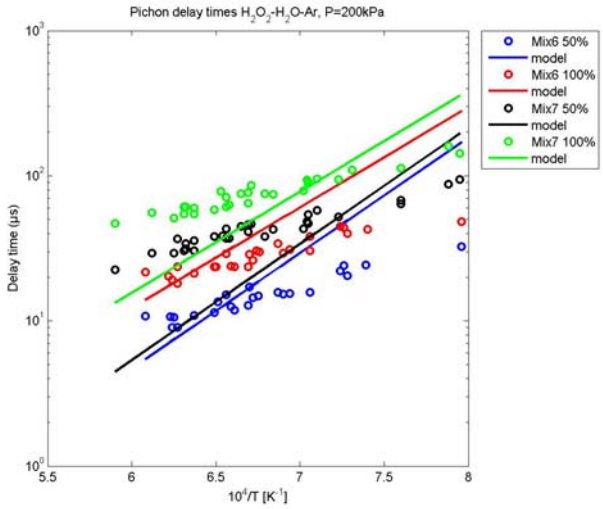

Figure S9: Experimental and calculated (Stanford) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

USC model:

Mean error =103 %

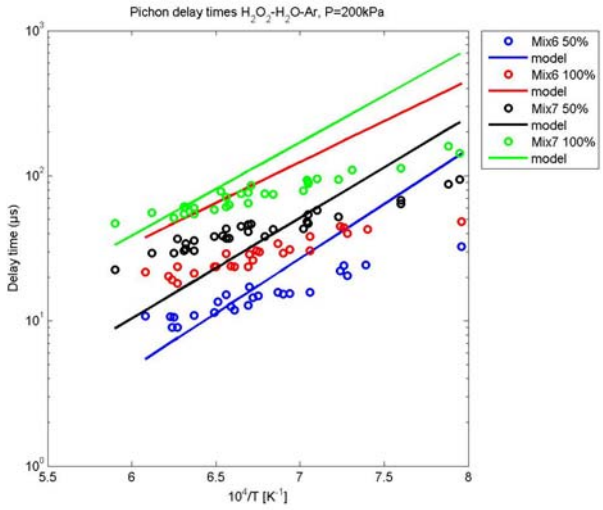

Figure S10: Experimental and calculated (USC) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

GRI model:

Mean error =87 %

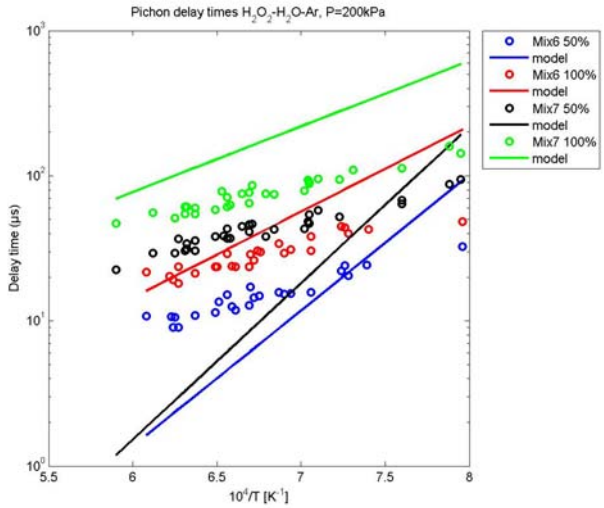

Figure S11: Experimental and calculated (GRI) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

Dagaut model:

Mean error =85 %

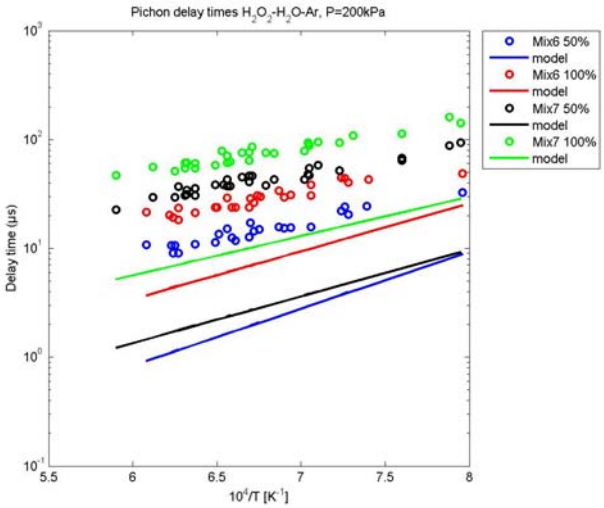

Figure S12: Experimental and calculated (Dagaut) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

Konnov model:

Mean error =86 %

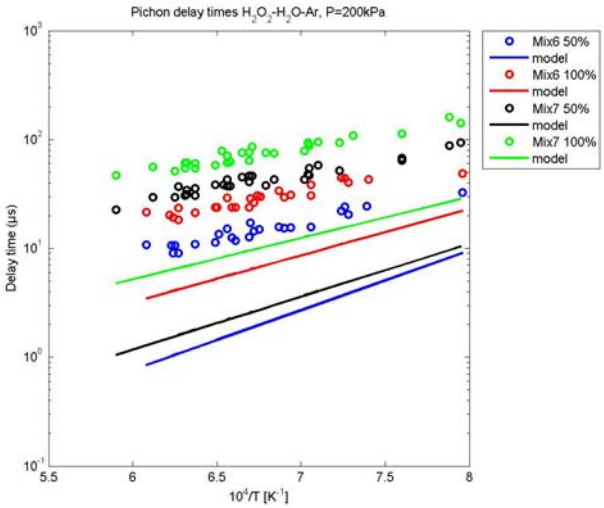

Figure S13: Experimental and calculated (Konnov) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

Present model:

Mean error =38 %

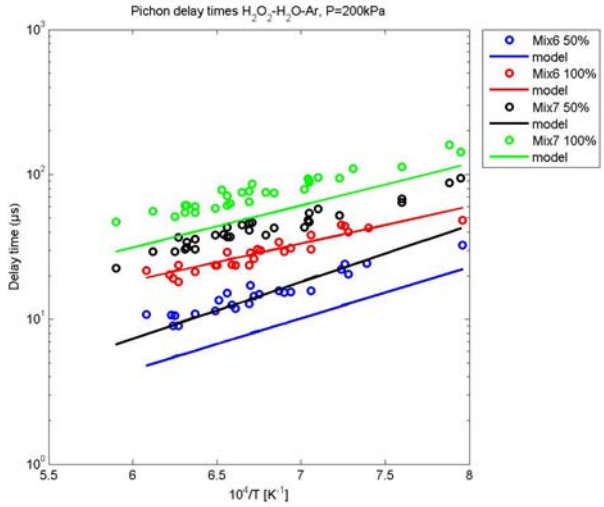

Figure S14: Experimental and calculated (Mevel) $\tau_{50\%}$ and $\tau_{100\%}$ for H_2O_2-H_2O-Ar mixtures.

Hydrogen-oxygen mixtures

Mixtures:
- N°1: X_{H2}=0.0169; X_{O2}=0.0081; X_{Ar}=0.975.
- N°2: X_{H2}=0.0200; X_{O2}=0.0050; X_{Ar}=0.975.

Delay-time definition:
The delay-time is defined as time to emission onset.

Stanford model:

Mean error =55 %

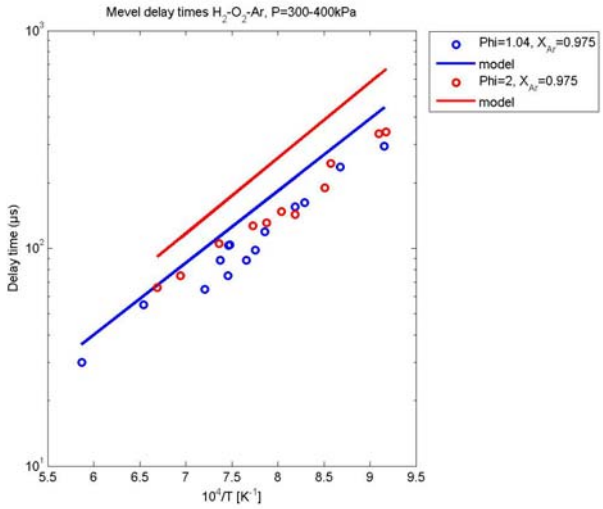

Figure S15: Experimental and calculated (Stanford) τ_{onset} for H_2-O_2-Ar mixtures.

USC model:

Mean error =42 %

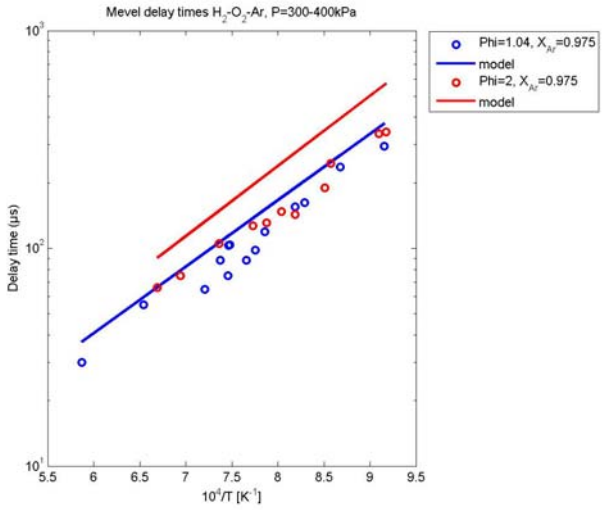

Figure S16: Experimental and calculated (USC) τ_{onset} for H_2-O_2-Ar mixtures.

GRI model:

Mean error =60 %

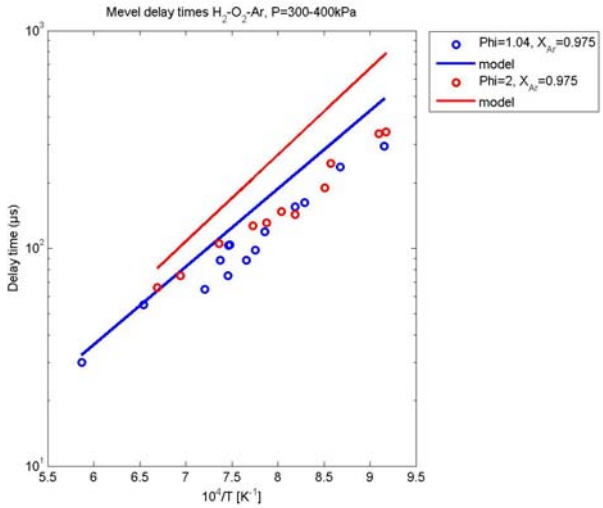

Figure S17: Experimental and calculated (GRI) τ_{onset} for H_2-O_2-Ar mixtures.

Dagaut model:

Mean error =28 %

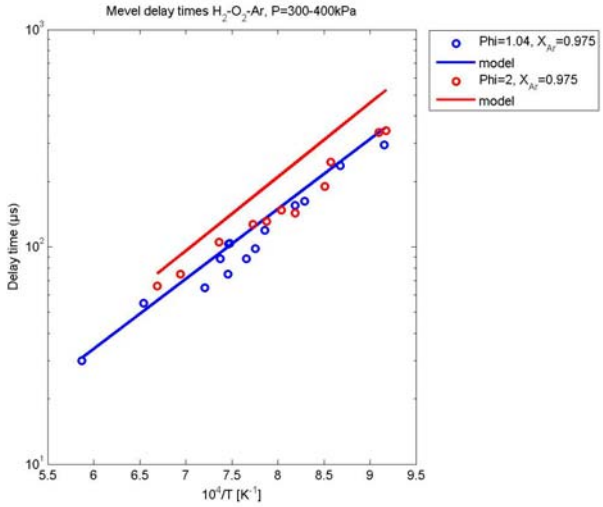

Figure S18: Experimental and calculated (Dagaut) τ_{onset} for H_2-O_2-Ar mixtures.

Konnov model:

Mean error =13 %

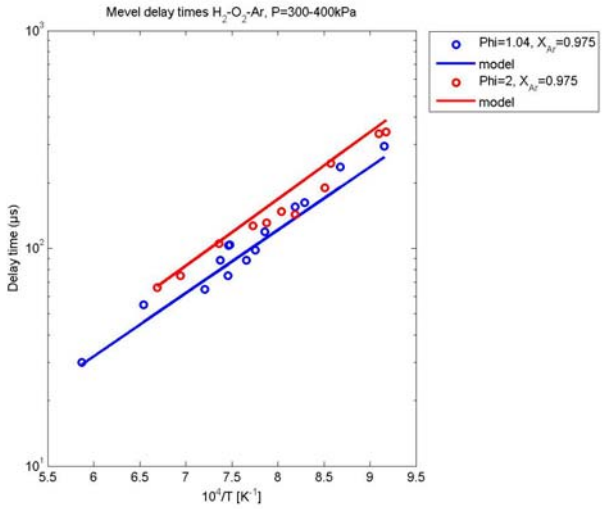

Figure S19: Experimental and calculated (Konnov) τ_{onset} for H_2-O_2-Ar mixtures.

Present model:

Mean error =13 %

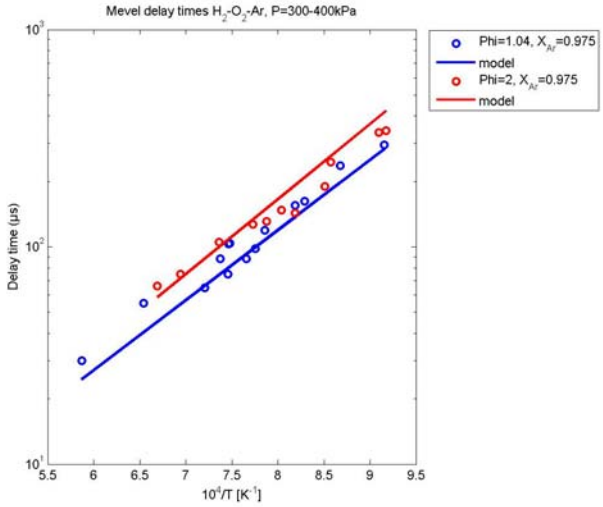

Figure S20: Experimental and calculated (Mevel) τ_{onset} for H_2-O_2-Ar mixtures.