Release of a preliminary best-to-use reaction mechanism for hydrogen combustion modelling

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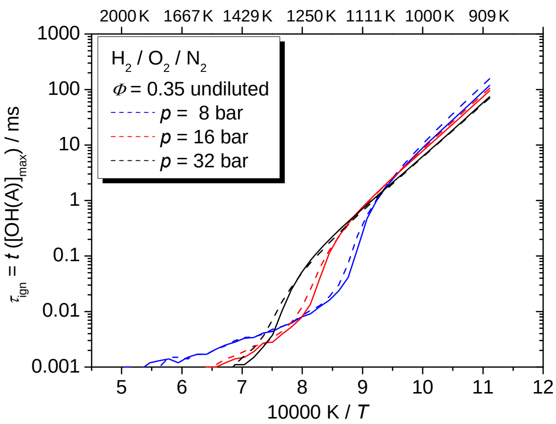
Release of a preliminary best-to-use reaction mechanism for hydrogen combustion modelling (DLR, TU/e**)**

Ignition delay of hydrogen rich fuels at GT relevant conditions have been studied in both a rapid compression machine (RCM) and a shock tube. Ignition delay times of undiluted hydrogen/oxygen mixtures as well as diluted mixtures with Argon or nitrogen were measured at pressures up to 32 bar, at equivalence ratios between Φ = 0.1 – 4.0 and at inlet temperatures higher than 900 K (see also table 1).

			Diluent		
Device	H_2	O_2	N_2	Ar	Φ
RCM	0.7	1.0	0.752	3.008	0.35
	0.7	1.0	3.76		0.35
	1.0	1.0	0.752	3.008	0.5
	1.0	1.0	3.76		0.5
	1.0	1.0	13.4	13.4	0.5
Shock Tube	1.0	1.0	26.8		0.5
	0.2	1.0		23.6	0.1
	0.2	1.0		3.76	0.1
	1.0	1.0		26.8	0.5
	2.0	1.0		30.8	1.0
	8.0	1.0		54.8	4.0

Tab. 1: Investigated mixture compositions for hydrogen ignition delay time experiments

The experimental results show that the ignition times for hydrogen mixtures are highly dependant on both temperature and pressure. The ignition delays measured in both the RCM and shock tube are in agreement with each other. Several kinetic mechanisms available in the literature as well as from NUI Galway and TU/e were tested against the experimental results. There predictions are in good agreement with measurements performed as published. For a more detailed discussion of the validation process see [3].



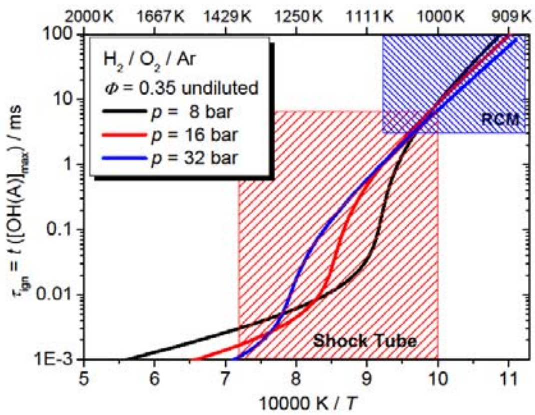
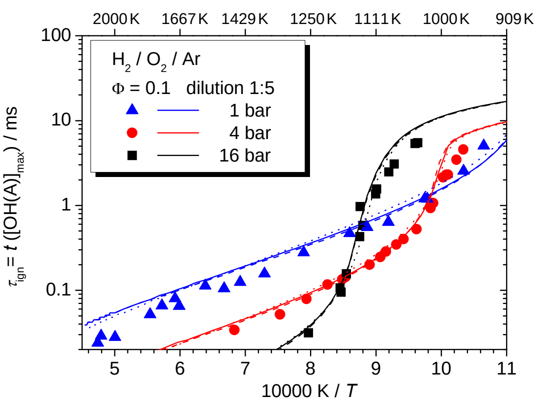


Fig 1: Comparison of ignition delay time predictions for $H_2/O_2/N_2$ undiluted blend. Solid line: reaction mechanism delivered by TU/e [4], dashed line: Keromnes et al., NUI Galway (01/2011) based on [1]

Fig 2: Validation regimes of RCM (blue hachures) at NUI Galway and shock tube measurements at DLR (red hachures, extrapolated for undiluted blend). Comparison of ignition delay time predictions for Li et al. [2] (solid line) and Keromnes et al., NUI Galway (01/2011) based on [1] (dashed line).



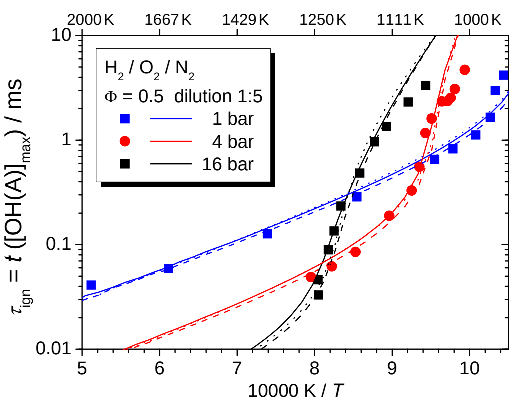


Fig. 3: Comparison of ignition delay time predictions for diluted $H_2/O_2/Ar$ mixture: full line – Keromnes et al., NUI Galway (01/2011) based on [1]; dashed line – Li et al. [2]; dotted line – TU/e [4]

Fig. 4: Comparison of ignition delay time predictions for diluted $H_2/O_2/N_2$ mixture: full line – Keromnes et al., NUI Galway (01/2011) based on [1]; dashed line – Li et al. [2]; dotted line – TU/e [4]

Comparison of the selected and project relevant H_2-reaction mechanisms (Keromnes et al. based on Ó Conaire et al. [1] from NUI Galway , Li et al. [2] and Konnov et al. from TU/e [4]) revealed only little differences with respect to the ignition delay time predictions at the conditions tested, see figures 1- 4. As an example calculations with the different mechanisms are also shown for typical conditions of the RCM experiments (H_2 / O_2 / (N_2 or Ar) - mixtures at Φ = 0.35 for different pressures), as sketched in figures 1 and 2. A further example is presented in figures 3 and 4, where experimental ignition delay times determined in a shock tube at DLR (H_2 / O_2 / (N_2 or Ar) mixture, Φ = 0.1 and 0.5, dilution 1:5, p = 1, 4 and 16 bar) are compared to the predictions of the different mechanisms. Therefore, all selected H_2/O_2-mechanisms are recommended so far as "best-to-use" reaction mechanism for H_2 / O_2 / (N_2 or Ar) combustion simulation based on ignition delay time validation experiments.

References:

[1] Ó Conaire, M., H. J. Curran, J. M. Simmie, W. J. Pitz and C. K. Westbrook, "A comprehensive modeling study of hydrogen oxidation." International Journal of Chemical Kinetics, 36 (2004) 603-622.

[2] Li, J., Zhao, Z. W., Kazakov, A., Chaos, M., Dryer, F. L. and Scire, J. J., "A comprehensive kinetic mechanism for CO, CH_2O, and CH_3OH combustion." International Journal of Chemical Kinetics, 39 (2007) 109-136.

[3] Keromnes, Alan, Donohoe, Nicola, Curran, Henry, Herzler, Jürgen, Naumann, Clemens and Griebel, Peter, "Ignition Delay Time Measurements and Validation of Reaction Mechanism for Hydrogen at Gas Turbine Relevant Conditions". In: Proceedings. The Future of Gas Turbine Technology, 5th International Conference, 27.-28.10.2010, Brussels, Belgium.

[4] Konnov et al., H2/air+NOx - reaction mechanism from January 27th, 2011, TU Eindhoven within H2-IGCC (2011)