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Numerical simulation of the impact of spark parameters on the ignition of ammonia/hydrogen/air mixtures

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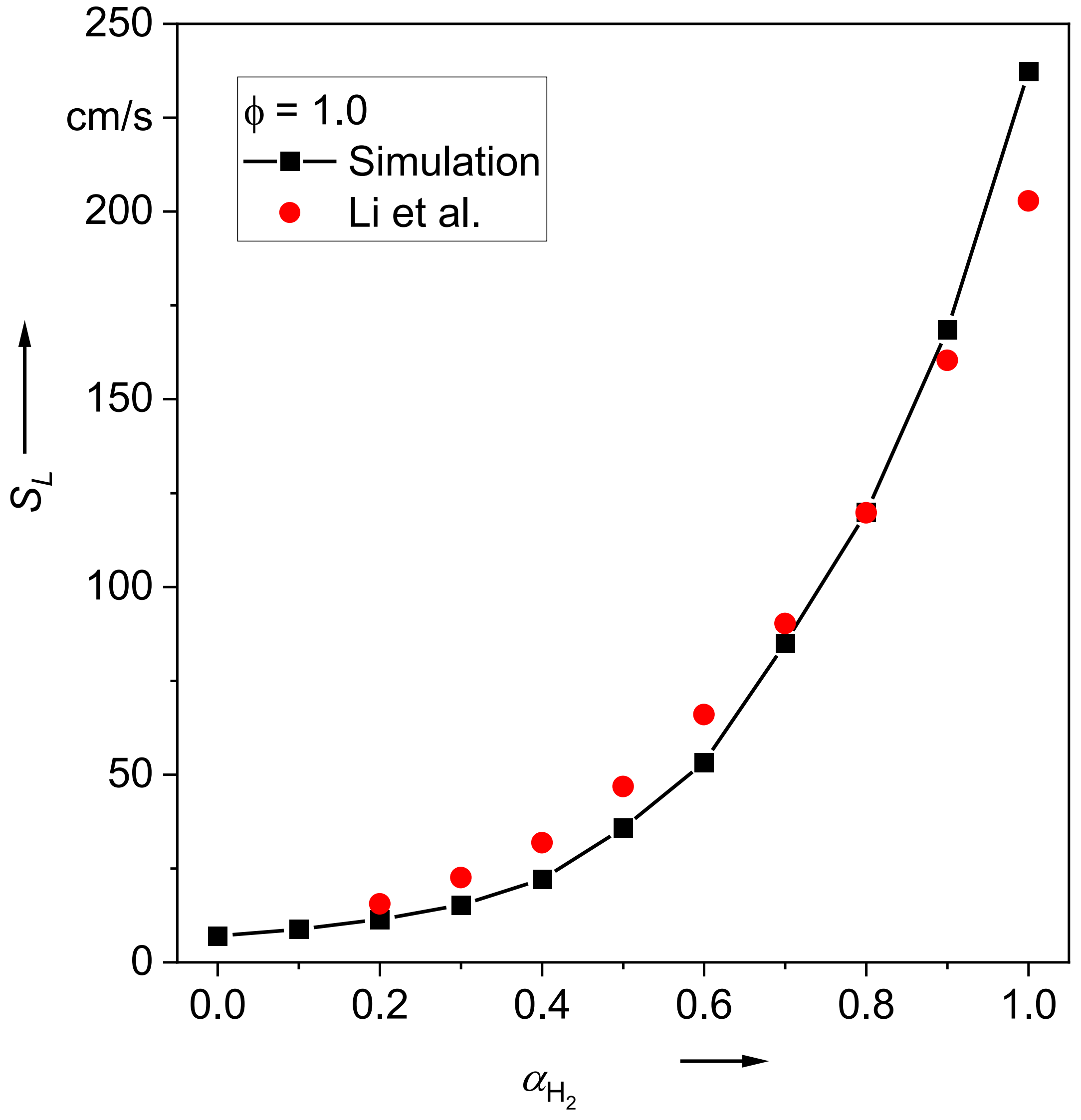
Motivation

- Usage of ammonia as a carbon-free fuel
  - Low laminar burning velocity
  - High ignition energy
- Hydrogen blending
  - α_{H_2}: fraction of hydrogen in the fuel
    - $\alpha_{H_2} = \frac{n_{H_2}}{n_{H_2} + n_{NH_3}}$
  - Increase in laminar burning velocity
  - Decrease in ignition energy
    - Comparison of experimental and numerical data



Scope of this work

- Investigate the ignition energy of various ammonia/hydrogen/air mixtures depending on
  - Geometry of numerical model
  - Different pressure assumptions (presence of pressure waves)
  - Source radii
  - Source times

- Comparison with experimental data [1]

	NH_3	H_2
Max. explosion pressure	6.9 bar	8.3 bar
Most ignitable mixture	20 vol%	22 vol%
Lower explosion limit	14 vol%	4 vol%
Upper explosion limit	32.5 vol%	77 vol%
Minimum ignition energy	14 mJ	0.017 mJ

Chemsafe Database [2]

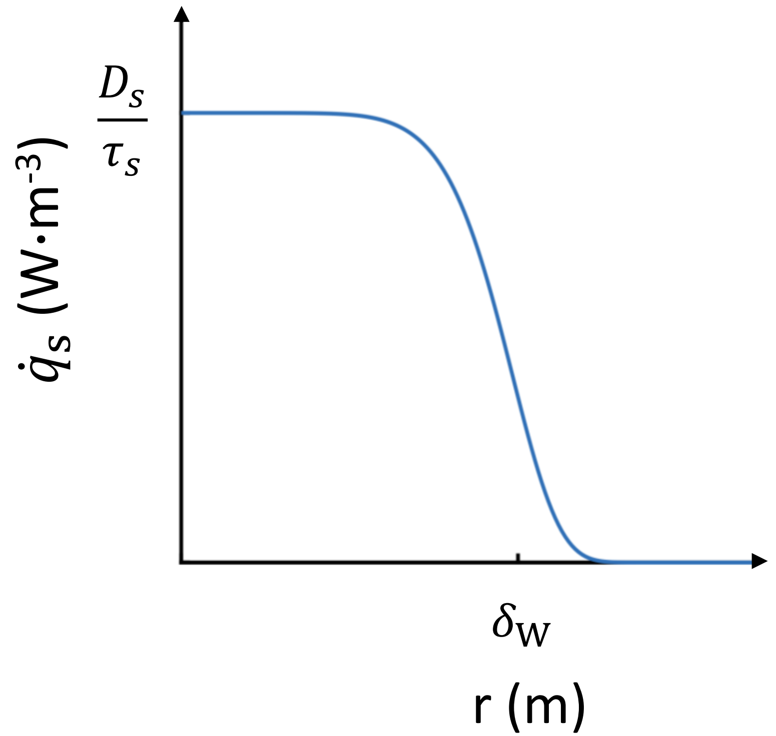
[1]: Essmann, S. et al. Ignition characteristics of hydrogen-enriched ammonia/air mixtures. **2024**
[2]: Chemsafe database, https://www.chemsafe.ptb.de

Simulation (In-House code INSFLA [3])

- Cylindrical & spherical geometry (1D, spatial coordinate is radius)
- Adaptive grid and time steps (time steps coupled to error control)
- Detailed molecular transport model including differential diffusion & thermal diffusion (Soret effect)
- Detailed reaction kinetics (mechanism from Shrestha et al. [4])
- Ignition source term given by

$$\dot{q}_s(r,t) = \frac{D_s}{\tau_s} \exp\left[-\left(\frac{r}{\delta_W}\right)^8\right]$$

  - D_s: source density
  - τ_s: source time
  - δ_w: source radius
  - r: radius
  - t: time
- For $t > \tau_s,\ \dot{q}_s = 0$



[3]: Maas, U., J. Warnatz Ignition processes in hydrogen oxygen mixtures. **1988**
[4]: Shrestha, K.P. et al. Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides. **2018**

Simulation | Choice of Parameters

Gas mixture

- NH_3: MIE at $\phi = 0.9$
- H_2: MIE at $\phi = 0.7$, but ignition limit curve is very flat between $\phi = 0.7$ and $\phi = 1.0$
- ➔ **keep $\boldsymbol{\phi = 0.9}$ constant, $\boldsymbol{\alpha_{H_2} = 0 \dots 0.2}$**
- Experimental data for comparison available at PTB [2]

Source radius

- Cylindrical simulation: Initial flame kernel measured in experiment with schlieren images (depending on α_{H_2})
- Spherical simulation: Calculation of spherical radius under the assumption that the ignition volume is constant

- $\alpha_{H_2} = 0$
  - $r_{0,\,cyl} = 2.64$ mm
  - $r_{0,\,sph} = 2.77$ mm

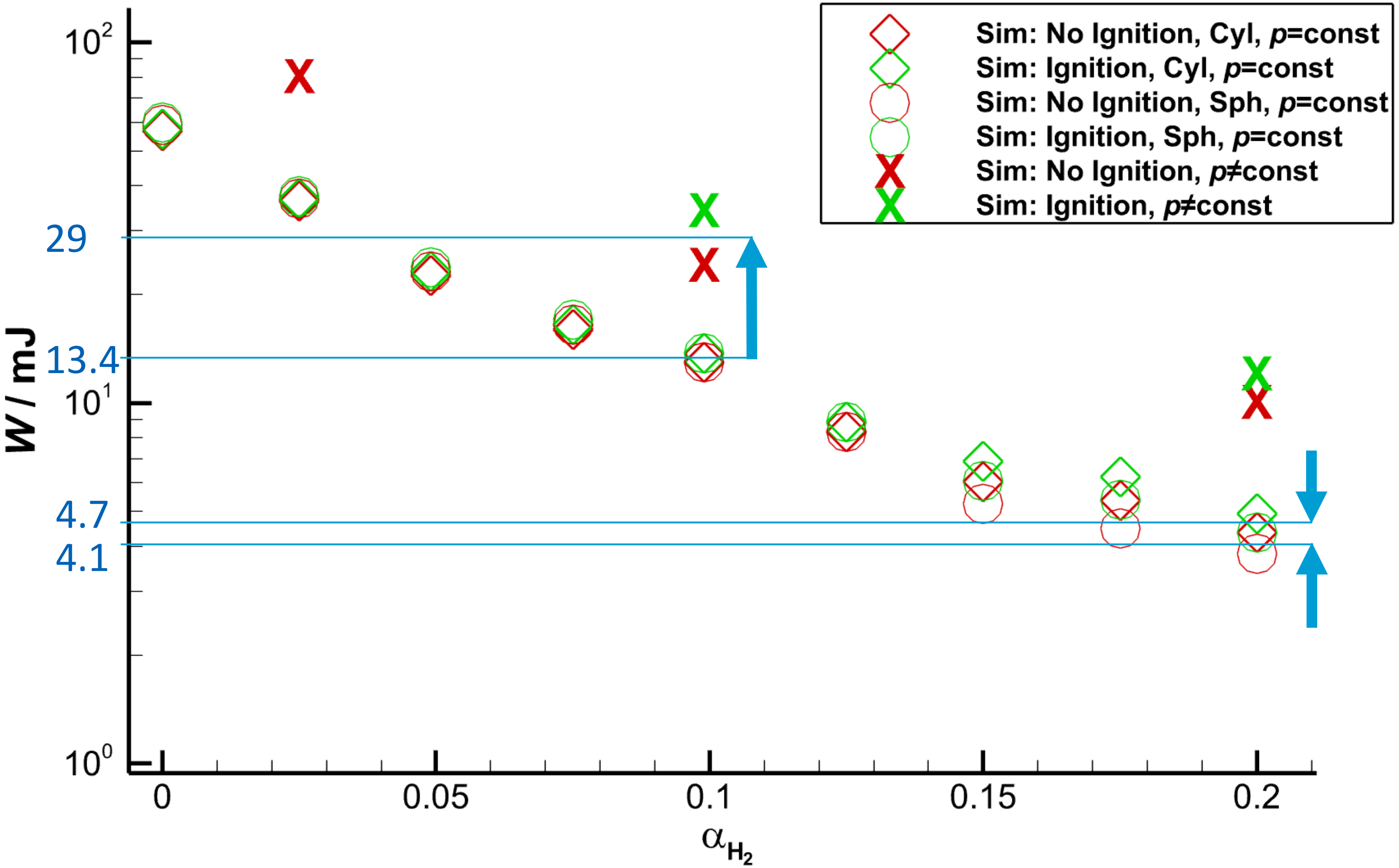
- $\alpha_{H_2} = 0.049$
  - $r_{0,\,cyl} = 1.69$ mm
  - $r_{0,\,sph} = 2.06$ mm

- $\alpha_{H_2} = 0.099$
  - $r_{0,\,cyl} = 1.28$ mm
  - $r_{0,\,sph} = 1.71$ mm

[2]: Essmann, S. et al. Ignition characteristics of hydrogen-enriched ammonia/air mixtures. **2024**

Results | Effect of Geometry & Shockwaves

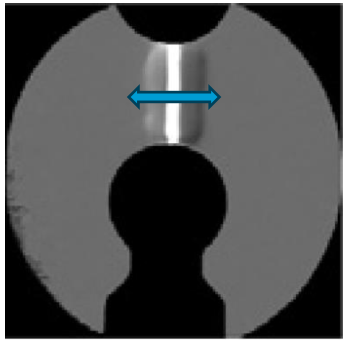
- Only minor differences with spherical geometry
  - Transport processes are not affecting the ignition
- In fully compressible simulation ($p \neq$ const) formation of pressure wave leads to higher ignition energies
  - Lower temperature in source volume when pressure wave is formed
- Constant pressure assumption is not valid with source times of τ_s = 10^{-6} s
  - Effect of shock wave needs to be considered

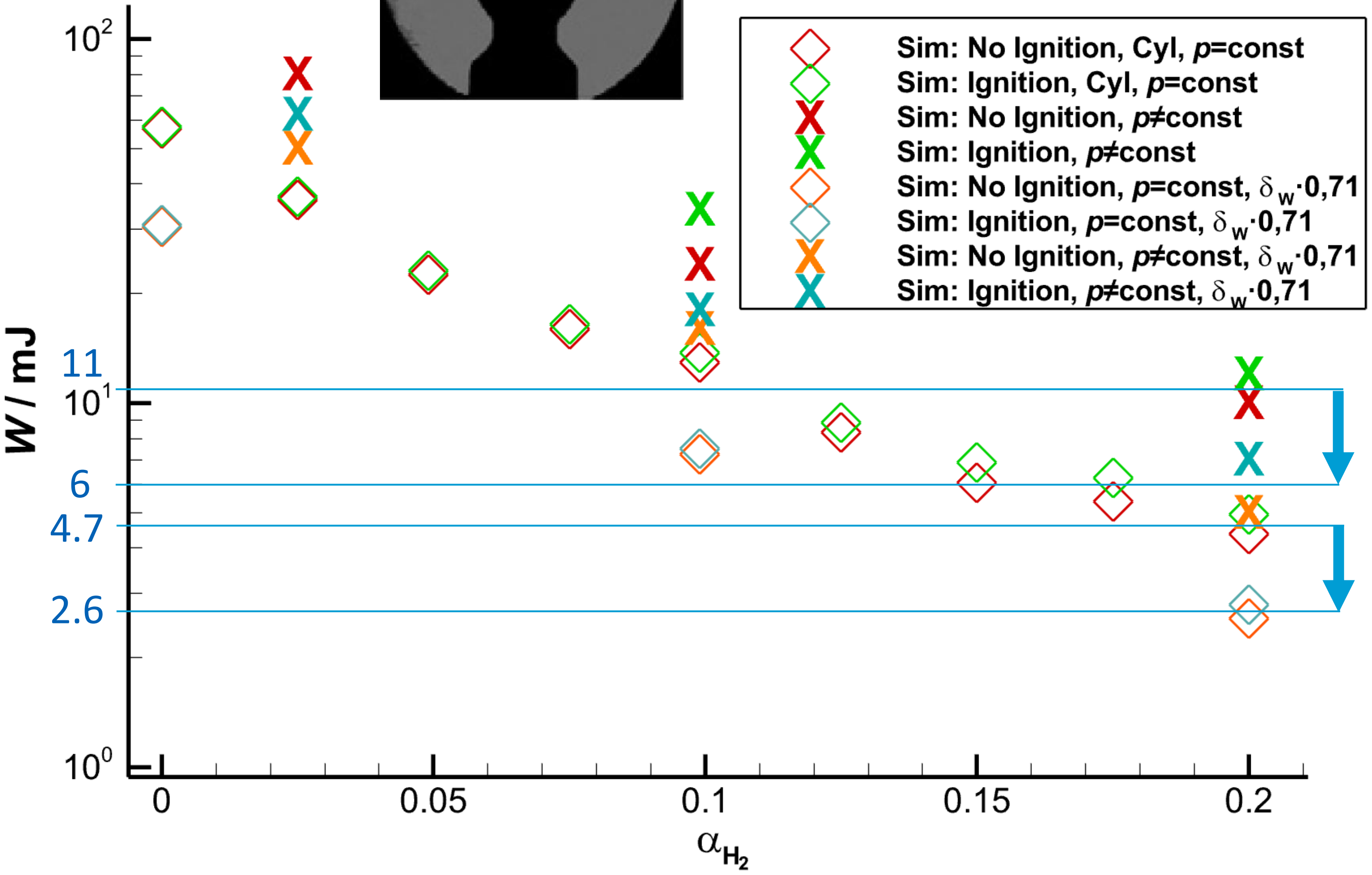


Ignition and no-ignition events for various α_{H_2}, comparison between simulations with spherical & cylindrical geometry, p = const & $p \neq$ const ($\tau_s = 10^{-6}$ s).

Results | Effect of Source Radius

- 29 % smaller source radii (this corresponds to a measurement error of approx. 40 % in the experiment) result in significantly lower ignition energy (≈ 45 % lower)
  - Higher energy density leads to a higher temperature in the source volume
- Similar decrease in minimum ignition energy for simulation with constant pressure and without





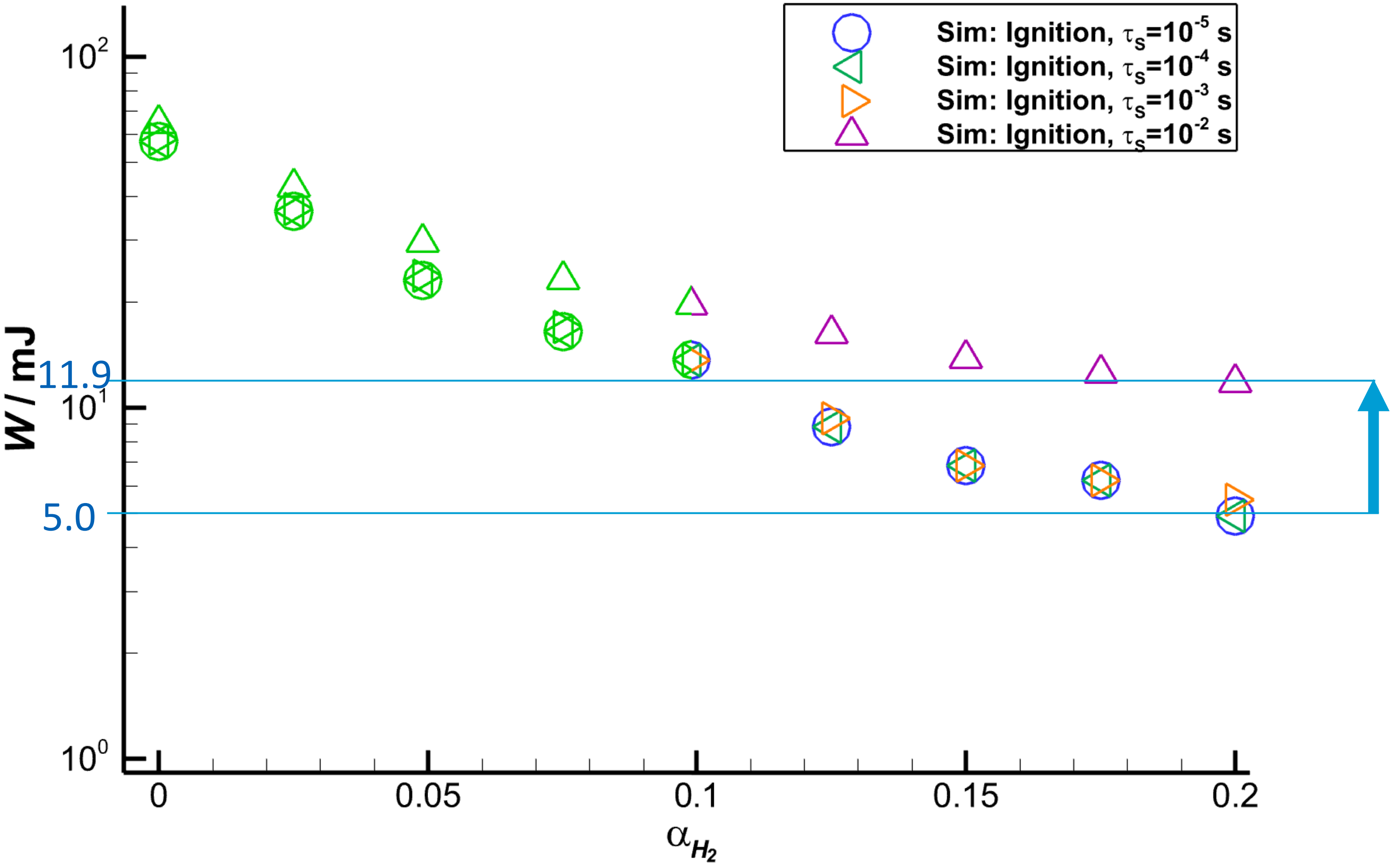
Ignition and no-ignition events for various α_{H_2}, comparison between simulations with radii measured in experiment (δ_w) and 29 % smaller radii ($\delta_w \cdot 0.29$).

PTB KIT Karlsruher Institut für Technologie

Results | Effect of Source Time

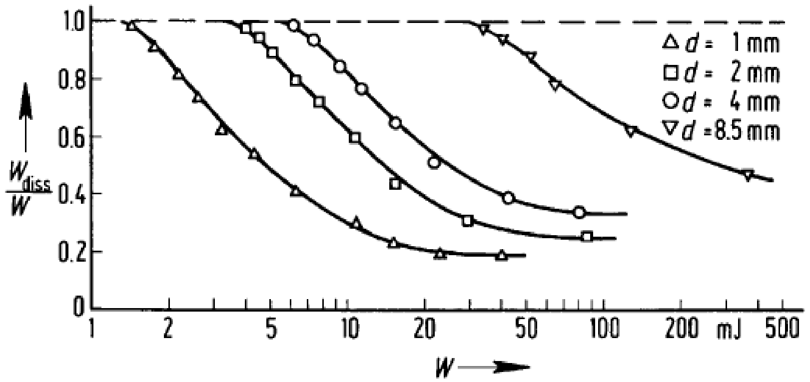
- For $\tau_s \leq 10^{-3}$ s mixtures with larger α_{H_2} show more dominant increase of ignition energy
  - H radicals generated by hydrogen combustion are diffusive and more dominant with greater H_2 content

- Shock waves are not formed, source time duration does not affect minimum ignition energy for $\tau_s \leq 10^{-3}$ s
  - Diffusion and heat conduction processes are on larger time scale and therefore not important
- For $\tau_s > 10^{-3}$ s more energy needed for ignition
  - Temperature decrease due to transport processes

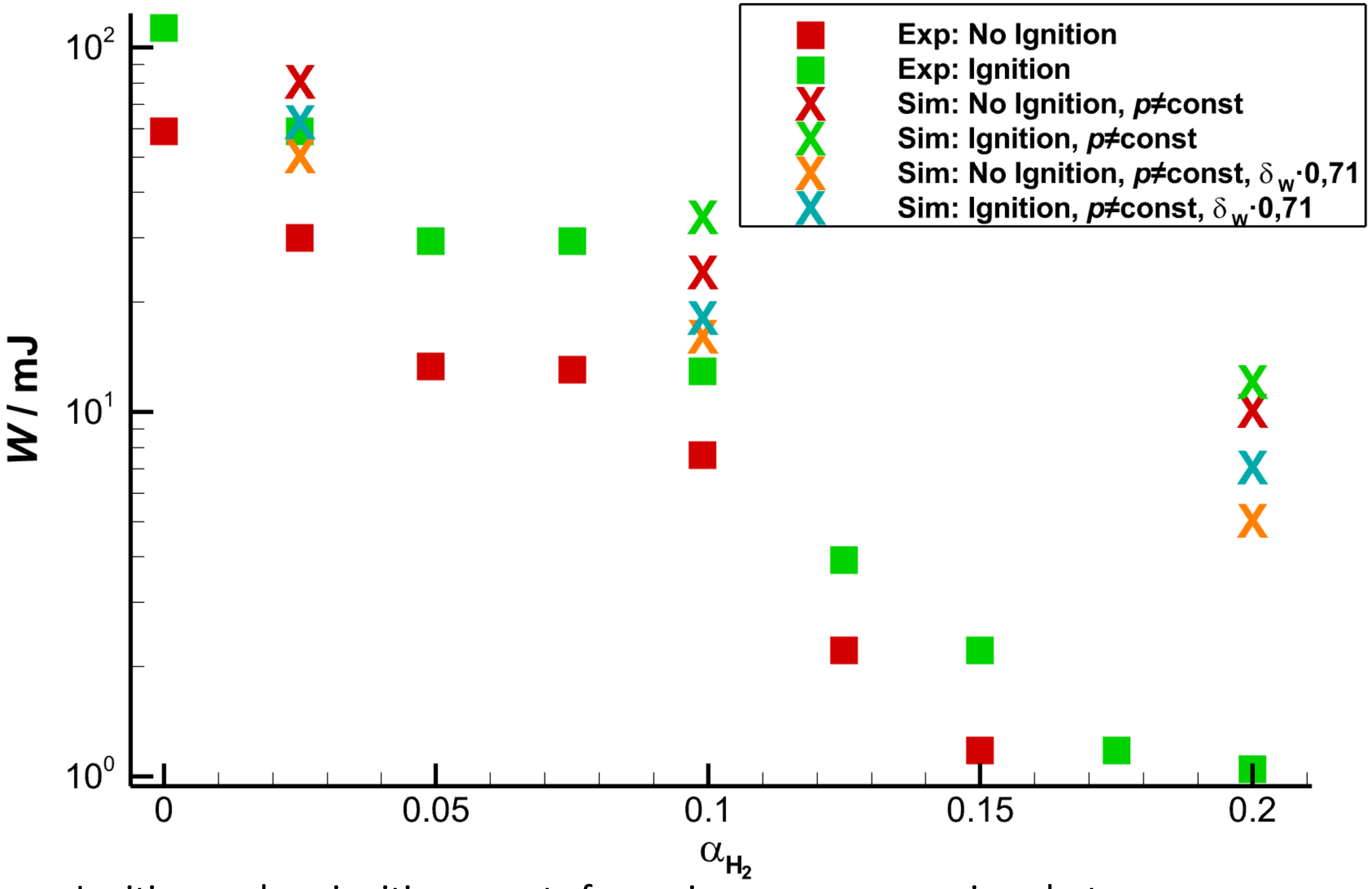


Ignition and no-ignition events for various α_{H_2}, comparison between simulations with different source times (p = const). No-ignition events are within a 1 mJ range.

Results | Comparison With Experiment



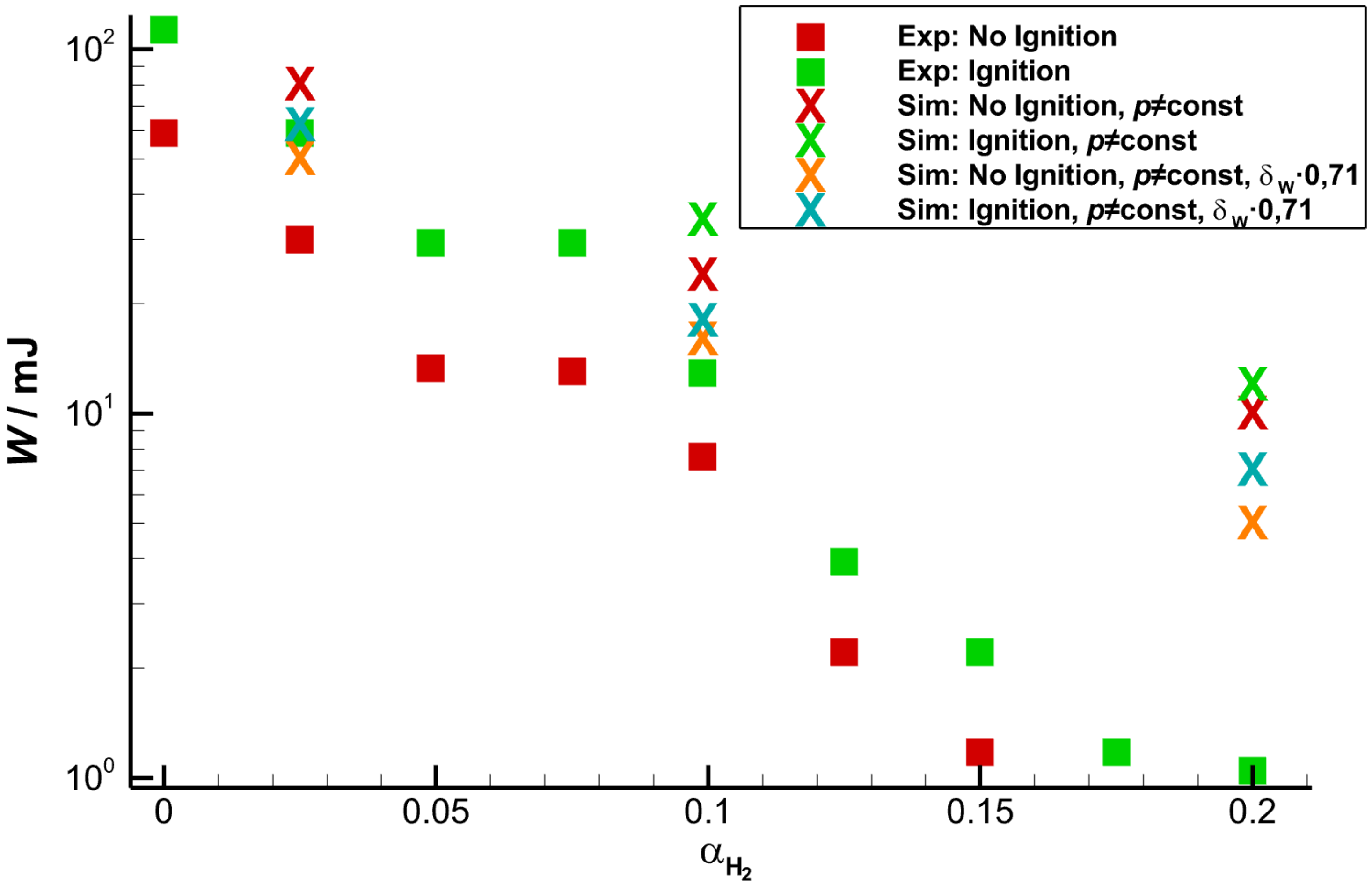
- For high energies overestimation of minimum ignition energy in experiment is likely
  - Energy transfer from capacitive discharge ($W = 1/2\, CV^2$) less efficient when energy increases



Ignition and no-ignition events for various α_{H_2}, comparison between simulations and experiment.

Results | Comparison With Experiment

- Chemical kinetics may introduce uncertainties for mixtures that deviate from pure ammonia or hydrogen
- Source radius measured in experiment with schlieren images is source radius for simulation and contains uncertainties
  - Source radius has significant effect on ignition energy



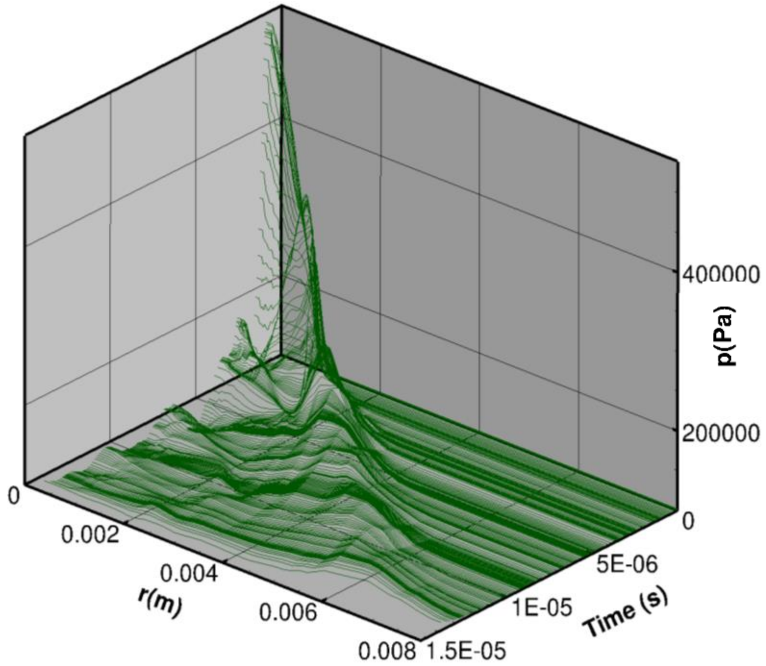
Ignition and no-ignition events for various α_{H_2}, comparison between simulations and experiment.

Conclusions

This work

- Simulations conducted with a fuel/air equivalence ratio (ϕ) of 0.9 & hydrogen addition up to $\alpha_{H_2} = 0.2$
- Geometry, pressure assumption, source radii and source time varied

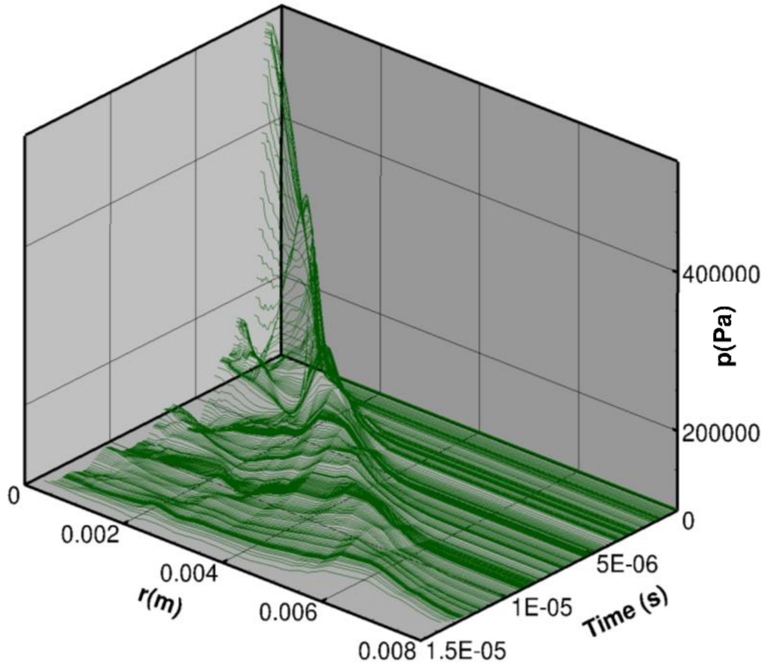
- Transport processes not important for source times $\leq 10^{-3}$ s
- Formation of pressure waves for short source times ($\tau_s \leq 10^{-6}$ s) lead to higher minimum ignition energies
- Source radii affects the minimum ignition energy significantly
- Comparison with experimental results
  - Trend of reduced minimum ignition energy is reflected by simulation
  - Experimental trend reflected by simulation results
    - Energy transfer from capacitive discharge less efficient when energy increases
    - Chemical kinetics may introduce uncertainties for mixtures that deviate from pure NH_3 or H_2



Pressure profile of simulation with p ≠ const and $\tau_s = 10^{-6}$ s

Outlook

- Simulation
  - Investigation of different reaction mechanisms
  - Modelling of the ionization process
- Experiment
  - Investigations with higher H_2 content planned
  - Optimization of radius measurement accuracy



Pressure profile of simulation with p ≠ const and $\tau_s = 10^{-6}$ s

THANK YOU

Any questions?

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