Numerical Simulation of the Impact of Spark Parameters on the Ignition of NH_3/H_2/Air Mixtures

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Motivation

- Ammonia is a promising energy carrier and fuel due to its high energy density, lack of carbon atoms and existing infrastructure
- Combustion processes using ammonia suffer from its low laminar burning velocity and high ignition energy
- Hydrogen addition to the fuel is considered to improve ignition and burning characteristics

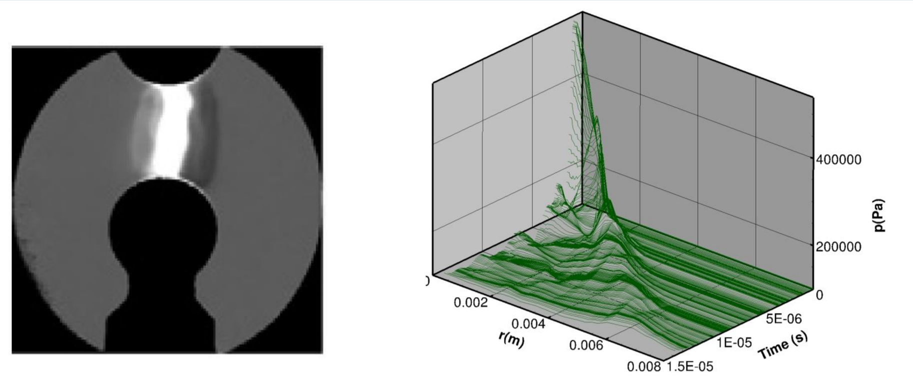

Fig. 1: Left: Schlieren image of spark-ignition [3]. Right: Pressure profile of ignition.

Numerical Method

In-House Program INSFLA [1]

- Solves conservation equations for total mass, species mass, energy, and momentum in 1D configurations
- Detailed chemical kinetics, reaction mechanism by Shrestha [2]
- Detailed molecular transport model including thermal diffusion (Soret effect) and differential diffusion
- Spatial grid and time steps adaptive, time stepping coupled to error control
- Planar, cylindrical, spherical geometries can be studied
- Constant pressure (*p* = const) assumption simplifies equation system and reduce computational effort
- Fully compressible *(p ≠ const)* simulation for short ignition source times to capture pressure waves induced by ignition

Spark-Ignition Source Model

- 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 $t > \tau_s,\ \dot{q}_s = 0$

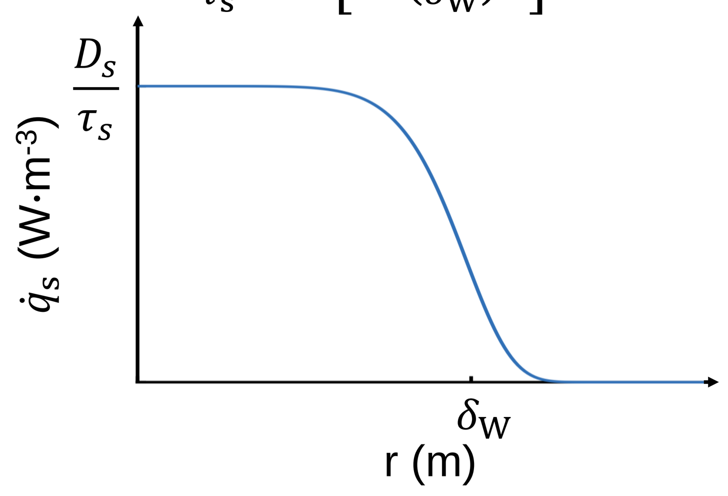

Fig. 2: Ignition source term $\dot{q}_s$ dependent of spatial coordinate *r*.

Determining the Source Radius

- Initial flame kernel radii (δ_w) measured in experiment with schlieren images [3]

Fig. 3: Schlieren image of the spark ignition for $\alpha = 0, \alpha = 0.05\ \alpha = 0.1$ [3]

α_{H_2}	δ_w / mm	$\delta_w \cdot 0.71$ / mm
0.000	2.640	1.885
0.025	2.119	1.514
0.049	1.686	1.204
0.075	1.420	1.014
0.099	1.276	0.911
0.125	1.029	0.735
0.150	0.859	0.613
0.175	0.814	0.582
0.200	0.744	0.531

Tab. 1: Source radii δ_w and reduced source radii $\delta_w \cdot 0.71$ depending on α_{H_2}

- Radius is dependent on the H_2 fraction in the fuel ($\alpha_{H_2} = \frac{n_{H_2}}{n_{NH_3}+n_{H_2}}$)
- Measured radius used for cylindrical simulations
- For spherical simulations, source radii calculated under the condition that the source volume is kept constant

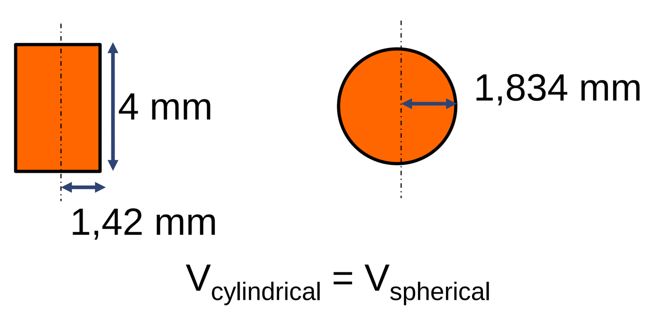

Fig. 4: Sketch of spherical radius determination

Results

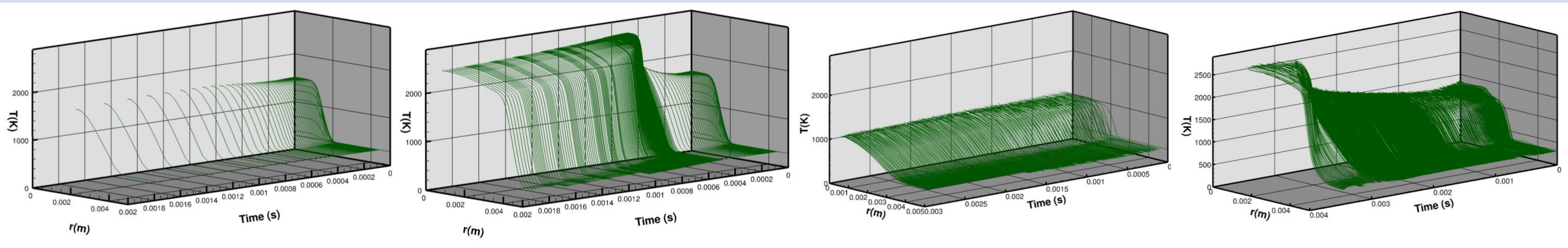

Fig. 5: Left: No-ignition & ignition for constant pressure simulation.
Right: No-ignition & ignition for fully compressible simulation

Effect of Source Time, Geometry & Pressure Waves

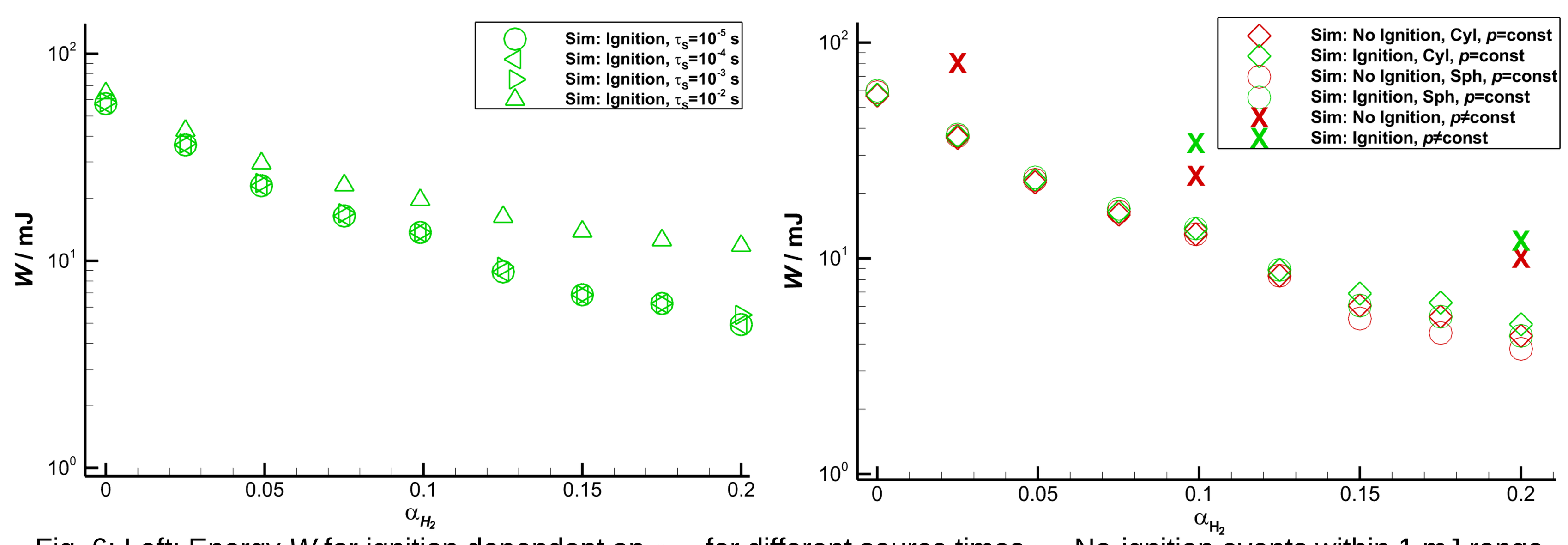

Fig. 6: Left: Energy *W* for ignition dependent on α_{H_2} for different source times τ_s. No-ignition events within 1 mJ range.
Right: Energy *W* dependent on α_{H_2} for different geometries and pressure assumptions for $\tau_s = 10^{-6}\ s$.

- Without presence of pressure waves, source time τ_s in the range of 10^{-5} s to 10^{-3} s does not affect ignition
- For $\tau_s > 10^{-3}$ s diffusion and heat conduction processes become important and minimum ignition energy increases
- In fully compressible simulation (*p* ≠ const) minimum ignition energy is higher because source energy partially expended on formation of pressure wave

Effect of Source Radius & Comparison with Experiment [3]

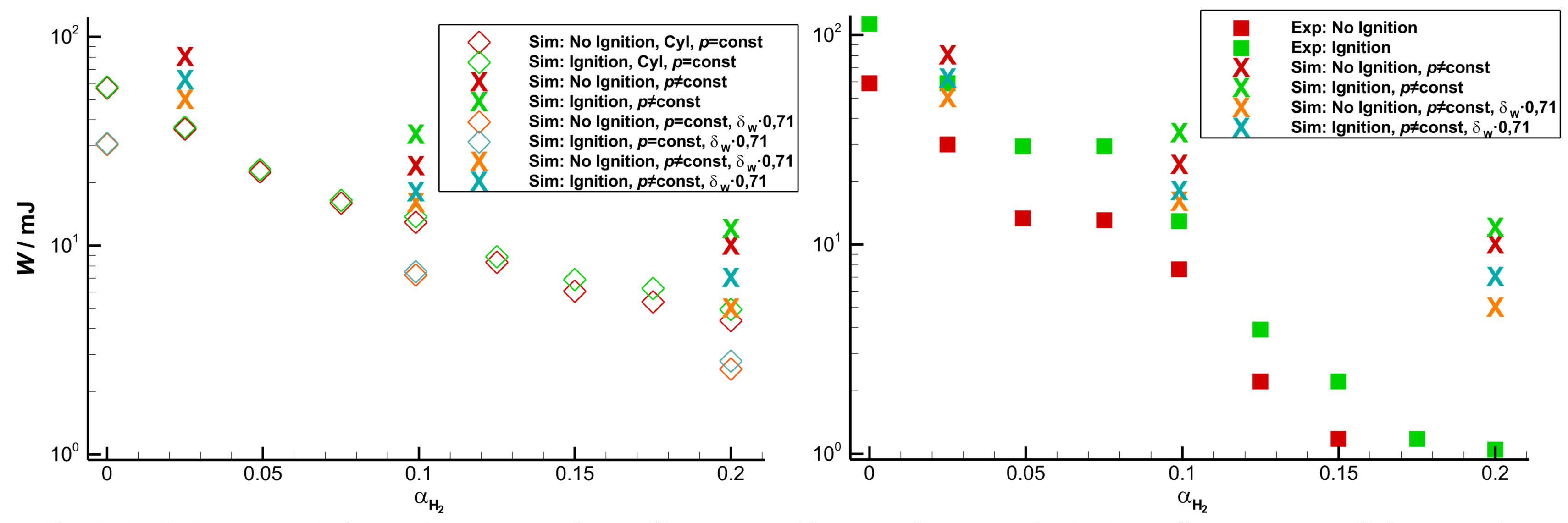

Fig. 7: Left: Energy *W* dependent on α_{H_2} for radii measured in experiment and 29 % smaller source radii ($\delta_w \cdot 0.71$).
Right: Comparison of simulation data (this work) and experimental data (from [3])

- Reducing the source radius increases the minimum ignition energy significantly
- Same trend in both, but in experiment more profound decrease in minimum ignition energy with increasing α_{H_2}
- Likely that experimental ignition energies indicated too high for small values of α_{H_2} because of inefficient capacitive discharge ($W = \frac{1}{2}CV^2$)
- Reaction mechanism may introduce uncertainties for mixtures that deviate from pure NH_3 or pure H_2
- Measurement error in determining initial flame kernel, resulting in inexact source radii in simulation

References

- [1] U. Maas, J. Warnatz, *Ignition processes in hydrogen-oxygen mixtures.* Combustion and Flame, 74(1), 1988, 53–69
- [2] K.P. Shrestha, L. Seidel, T. Zeuch, F. Mauss, *Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides*. Energy & Fuels, 32(10), 2018,10202–10217
- [3] S. Essmann, J. Dymke, J. Höltkemeier-Horstmann, D. Möckel, C. Schierding, M. Hilbert, C. Yu, U. Maas, D. Markus *Ignition characteristics of hydrogen-enriched ammonia/air mixtures*. Applications in Energy and Combustion Science 17, 2024

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