Numerical Investigation of the Minimum Ignition Energy in Ammonia/Hydrogen/Air Mixtures Considering Radiative Heat Loss

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Motivation

- Ammonia is a promising energy carrier and fuel due to its high volumetric energy density compared to hydrogen, 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
- Reliable ignition of mixtures important for technical applications
- Lack of knowledge on the ignition properties of NH3/H2 fuels, especially lean mixtures
- Low reactivity of ammonia makes ignition of these fuels prone to perturbation even by minor physical effects

→ Goal: investigate the effect of radiation on Minimum Ignition Energy MIE of NH_3/H_2/Air mixtures at the lean flammability limit

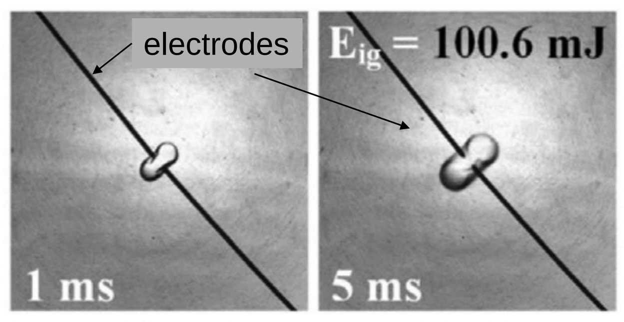

Fig. 1: Schlieren image of spark-ignition [5]; courtesy of Prof. S. Shy (NCU Taiwan)

Methodology

Approach

- Detailed numerical simulation study of ignition scenarios in 10%H_2 / 90%NH_3 (mol/mol) mixtures with air
  - Adjustable ignition source energy
  - Different equivalence ratios (from lean flammability limit to stoichiometric)
  - Radiation terms can be considered or neglected

In-House Program INSFLA [1] for ignition simulations

- Solves conservation equations for total mass, species mass, energy, and momentum in 1D configurations
- Detailed chemical kinetics, reaction mechanism by Glarborg [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
- Spherically symmetric configuration
- Constant pressure (p = const) assumption; accurate for source time durations above ≈ 20 µs [1]
- Optically thin approximation model (OTM) applied for radiative heat loss [3]

Spark-Ignition Source

- Volumetric ignition source
  - source time (500 µs in this work*)
  - source radius (1 mm in this work*)

Optically Thin Approximation Model (OTM)

- Volumetric radiative heat loss given by $\dot{q}_{rad} = 4 \cdot k \cdot \sigma \cdot (T^4 - T_b^4)$
  - k: total Planck mean absorption coefficient
  - σ: Stefan-Boltzmann constant
  - T: local temperature
  - T_b: background temperature (300 K in this work)

Simulation Setup & Evaluation Conditions

- Homogeneous NH_3/H_2/Air mixture with varrying equivalence ratio and fixed hydrogen content in the fuel ($a_{H_2} = \frac{n_{H_2}}{n_{H_2} + n_{NH_3}} = 0.1$)
- Atmospheric conditions: p = 1 bar, T = 300 K
- Successful ignition is counted when flame reaches r = 7.5 cm*
- Partially successful ignition counted when flame exists but not propagates until 7.5 cm

* Parameters based on experimental data for future comparison

- The flammability limit is at an equivalence ratio slightly below Φ = 0.5 – indicated by the orange bar, representing three distinct zones

I. Below the bar, the energy deposition does not lead to a propagating flame **(no ignition)**
II. Above the bar, the energy deposition leads to a stable propagating flame (**successful ignition**)
III. Within the region represented by the bar, a flame front forms and propagates outward initially, followed by extinction due to the radiative heat loss (**partially successful ignition**)

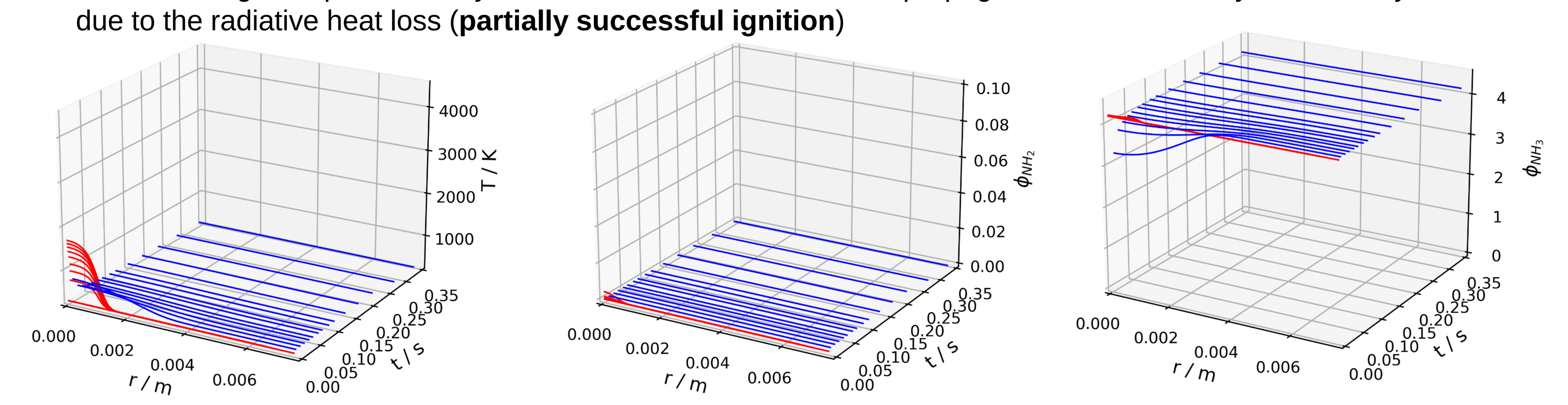

Fig. 4: **No ignition (I):** Calculated transient profiles for temperature (left), NH2 (middle) and NH3 (right) specific mole number ϕ (ratio of mass fraction to molar mass) for fuel/air equivalence ratio **Φ = 0.51** with source energy **3.0 mJ** and considering radiation

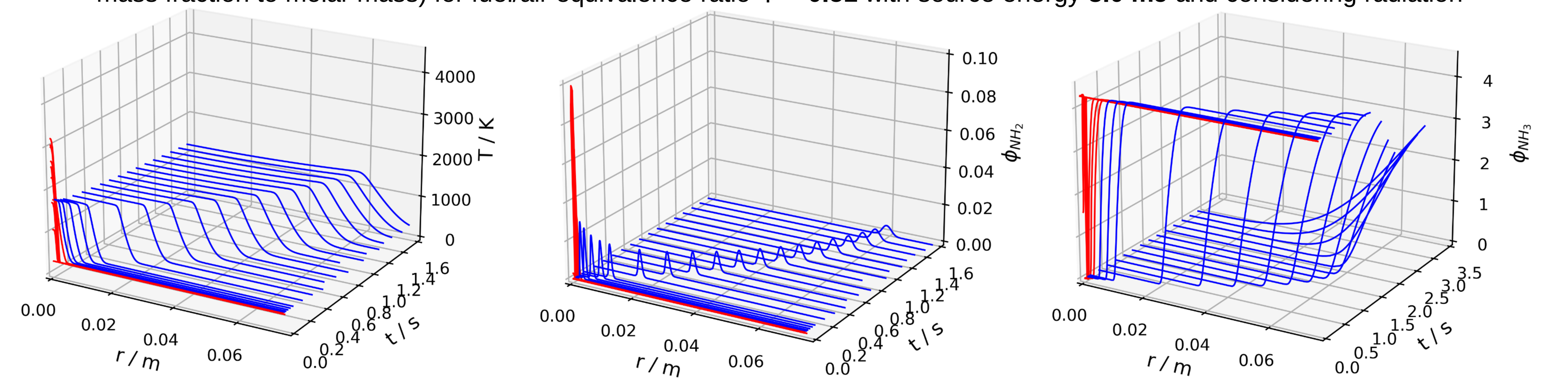

Fig. 5: **Successful ignition (II):** Calculated transient profiles for temperature (left), NH2 (middle) and NH3 (right) specific mole number ϕ (ratio of mass fraction to molar mass) for fuel/air equivalence ratio **Φ = 0.51** with source energy **3.8 mJ** and considering radiation

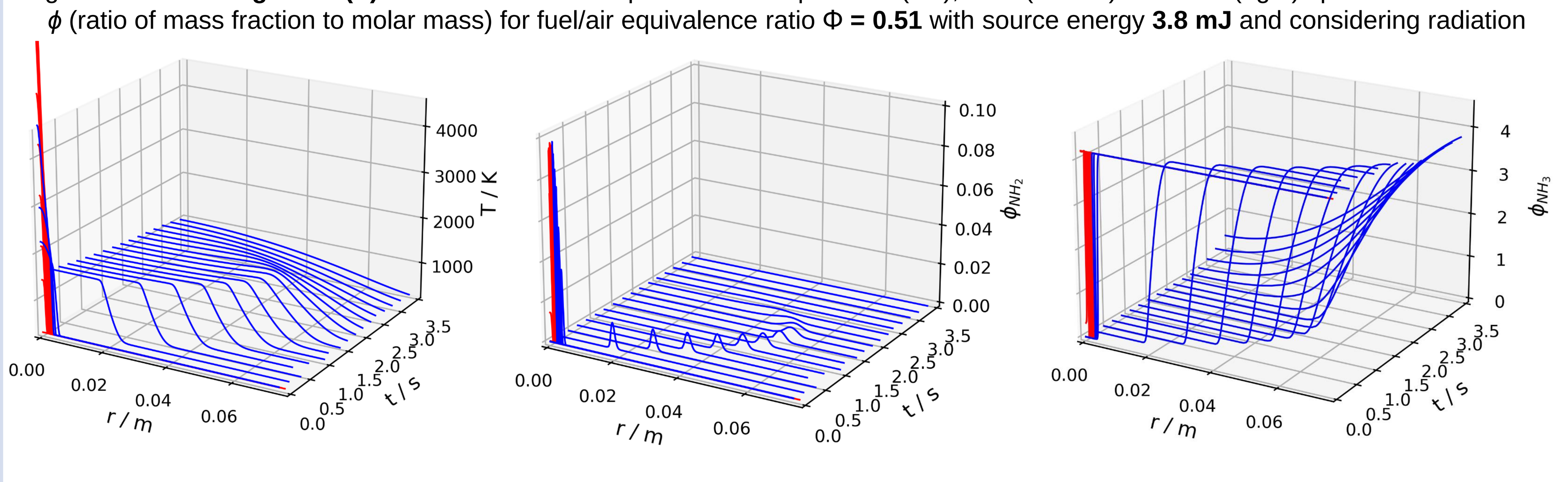

Fig. 6: **Partially successful ignition (III):** Calculated transient profiles for temperature (left), NH2 (middle) and NH3 (right) specific mole number ϕ (ratio of mass fraction to molar mass) for fuel/air equivalence ratio **Φ = 0.50** with source energy **41 mJ** and considering radiation

Fig. 4: No ignition (I)
- No propagating flame
- No NH_2 peak (correlates with position of heat release rate maximum) is traveling
- Only very small amount of NH_3 consumed during source energy deposition

Fig. 5: Successful ignition (II)
- Stable flame front forms and propagates outward after ignition
- NH_2 peak (correlates with position of heat release rate maximum) moves outward
- NH_3 is fully consumed by chemical reactions

Fig. 6: Partially successful ignition (III)
- Flame front forms but weakens due to radiative heat loss
- NH_2 peak initially moves outward but diminishes as temperature drops
- NH_3 not fully consumed, indicating extinction

Fig. 7 Comparison of NH2 peak of II and III:
- NH_2 peak position indicates location of the flame; slope shows flame speed
- In partially successful ignition, flame movement slows down and extinguishes

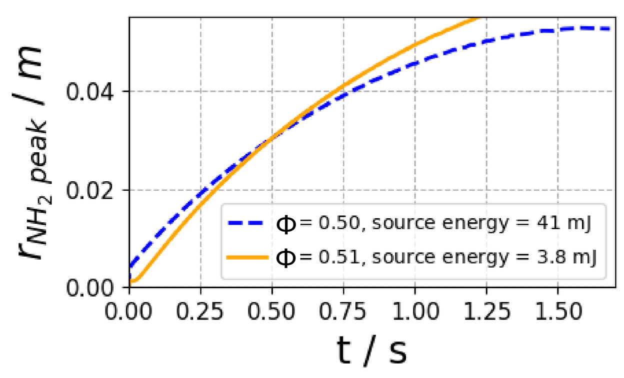

Fig. 7: Position of the NH_2 peak as a function of time for Φ = 0.51 (ignition energy = 3.8 mJ) and Φ = 0.50 (ignition energy = 41 mJ)

Results

Effect of Radiation on Minimum Ignition Energy (MIE)

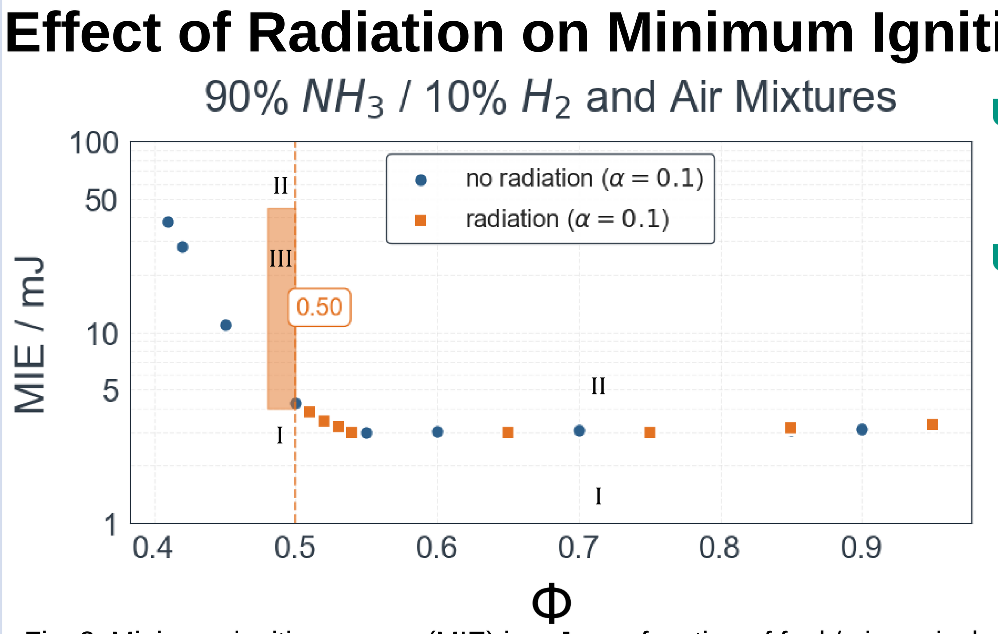

Fig. 2: Minimum ignition energy (MIE) in mJ as a function of fuel / air equivalence ratio Φ

- For 0.5 < Φ < 1.0 radiative heat loss has no appreciable effect on the ignition
- For 0.4 < Φ < 0.5 system is sensitive to radiation:
  - Radiation neglected: flame survives (II)
  - Radiation not neglected: flame starts propagating and finally extinguishes (III)

Conclusion

- It is clearly confirmed, that for the calculation of the MIE for lean mixtures close to the flammability limit (Φ < 0.5), radiation must not be neglected
- Radiation causes flame extinction even after several centimeters of flame propagation due to additional heat loss caused by radiation
- The values for the MIE are strongly depended of the criteria for defining a successful flame (see region I, II, III)
- At the flammability limit, the effect of radiative heat loss influences the MIE significantly

References

- [1] U. Maas, J. Warnatz, *Ignition processes in hydrogen-oxygen mixtures.* Combustion and Flame, 74(1), (1988), 53–69
- [2] J. Jian et al. *An experimental, theoretical, and kinetic modeling study of post-flame oxidation of ammonia*, Combustion and Flame 261 (2024)
- [3] M. Faghih et al. *Effect of radiation on laminar flame speed determination in spherically propagating NH3-air, NH3/CH4/air and NH3/H2-air flames at normal temperature and pressure*, Combustion and Flame 257 (2023)
- [4] H. Nakamura, M. Shindo, *Effects of radiation heat loss on laminar premixed ammonia/air flames*, Proceedings of the Combustion Institute 37 (2) (2019)
- [5] C. Wu et al. *Experimental and numerical investigation of the induced ignition process in ammonia/air and ammonia/hydrogen/air mixtures*, Proceedings of the Combustion Institute 40 (1-4) (2024)

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