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Characteristics of ammonia/hydrogen premixed combustion in a novel Linear Engine Generator

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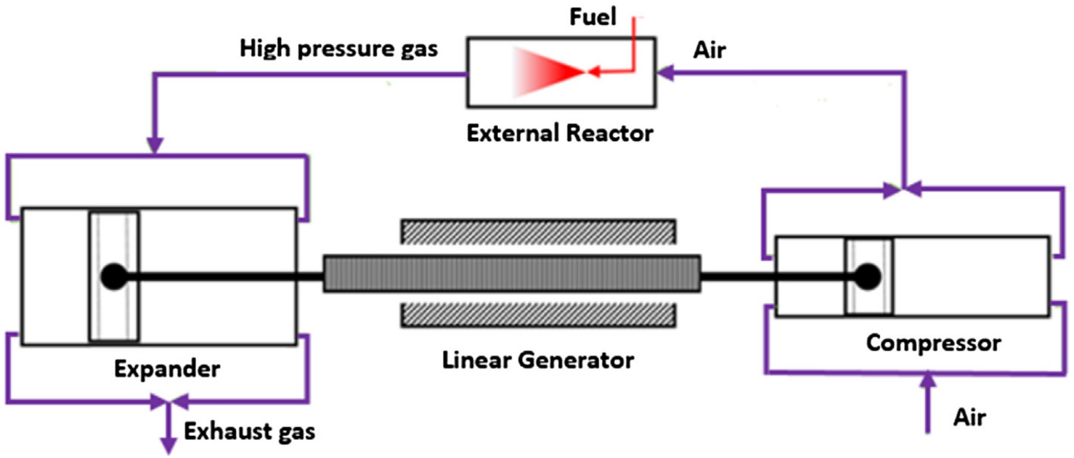
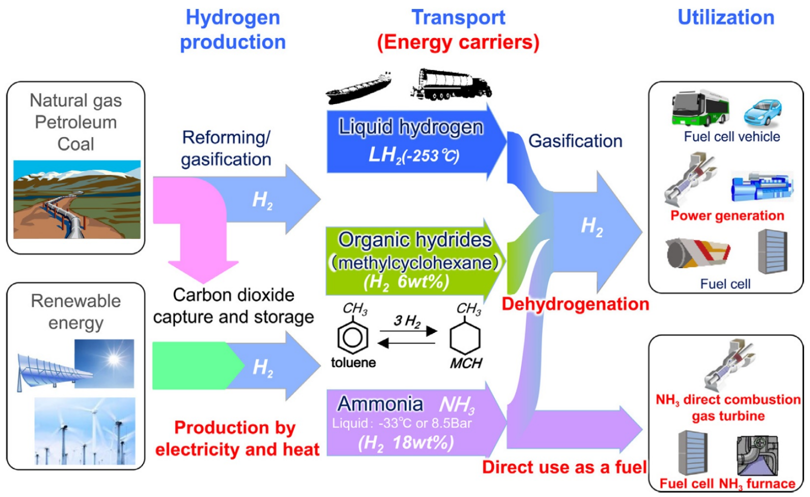
Introduction – background

- Linear Engine Generator (LEG) – a novel hybrid–powertrain solution
  - Simpler and more compact structure
  - Lower friction loss
  - More control freedom
  - Wider fuel adaptability
- Ammonia as a fuel – carbon-free alternative fuel and potential hydrogen carrier
  - High gravimetric and volumetric hydrogen density
  - Well-established industry of production, storage, transportation and utilization
  - Renewable production technologies are available





[1] Jia, B., et al., *Dynamic and thermodynamic characteristics of a linear Joule engine generator with different operating conditions.* Energy Conversion and Management, 2018. **173**: p. 375-382.

[2] Kobayashi, H., et al., *Science and technology of ammonia combustion.* Proceedings of the Combustion Institute, 2019. **37**(1): p. 109-133.

Introduction – objectives

- A more detailed and extensive investigation under engine-operation condition is still required to better support the combustion system of the target LEG prototype.
- Identify an ammonia chemical kinetic reaction mechanism
- Parametric study on the effects of equivalence ratio, hydrogen blending ratio, initial temperature and initial pressure on premixed laminar flame speed, ignition delay and flame species

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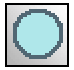
Methodology

ANSYS CHEMKIN PRO	
Premixed laminar flame speed modelling	
Ignition delay time modelling	
Burner-stabilized flame structure modelling	

◆ Mechanism selection

Chemical kinetic reaction mechanism
Otomo's mechanism[3]
Duynslaegher's mechanism[4]
Nakamura's mechanism[5]

◆ Parametric study

Factor	Range
Equivalence ratio	$0.8 - 1.6$
Hydrogen blending ratio	$0.0 - 0.6$
Initial temperature	$300 - 700\ K$
Initial pressure	$1 - 20\ bar$

[3] Otomo, J.; Koshi, M.; Mitsumori, T.; Iwasaki, H.; Yamada, K., Chemical kinetic modeling of ammonia 436 oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion. 437 *International Journal of Hydrogen Energy* **2018,** 43, (5), 3004-3014.
[4] Duynslaegher, C.; Contino, F.; Vandooren, J.; Jeanmart, H., Modeling of ammonia combustion at low 443 pressure. *Combustion and Flame* **2012,** 159, (9), 2799-2805.
[5] Nakamura, H.; Hasegawa, S.; Tezuka, T., Kinetic modeling of ammonia/air weak flames in a micro flow 461 reactor with a controlled temperature profile. *Combustion and Flame* **2017,** 185, 16-27.

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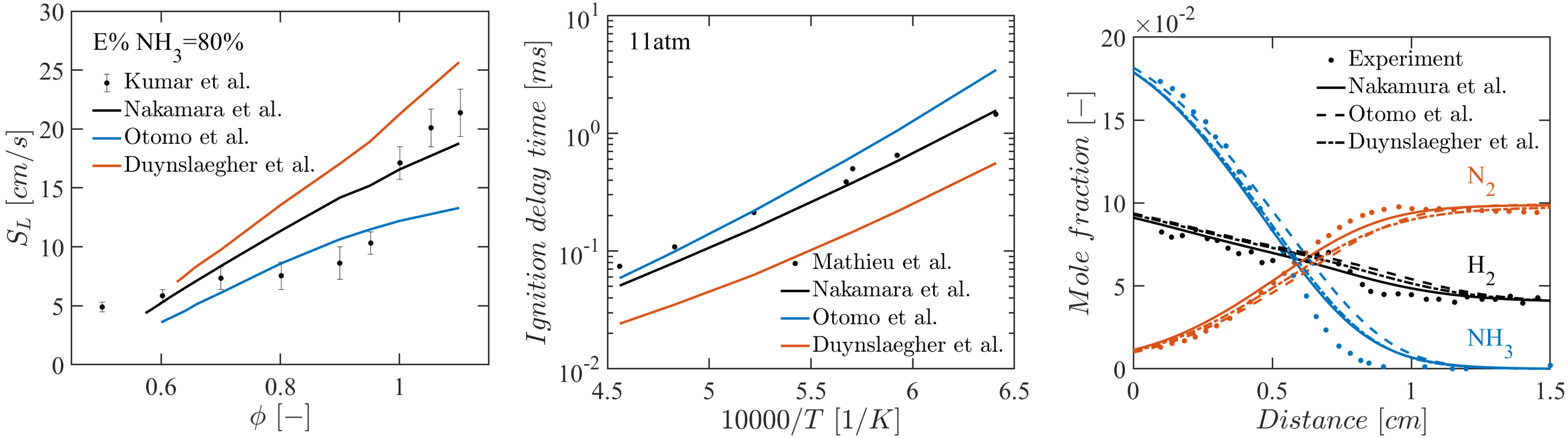
Mechanism selection

- Premixed laminar flame speed: $E\%NH_3 = 20\%,\ 50\%,\ 80\%$
- Ignition delay: $1.4, 11, 30\ atm$
- Main species: $NH_3, N_2, H_2, NO, N_2O, NH_2$

Chemical kinetic reaction mechanism
Otomo's mechanism
Duynslaegher's mechanism
Nakamura's mechanism



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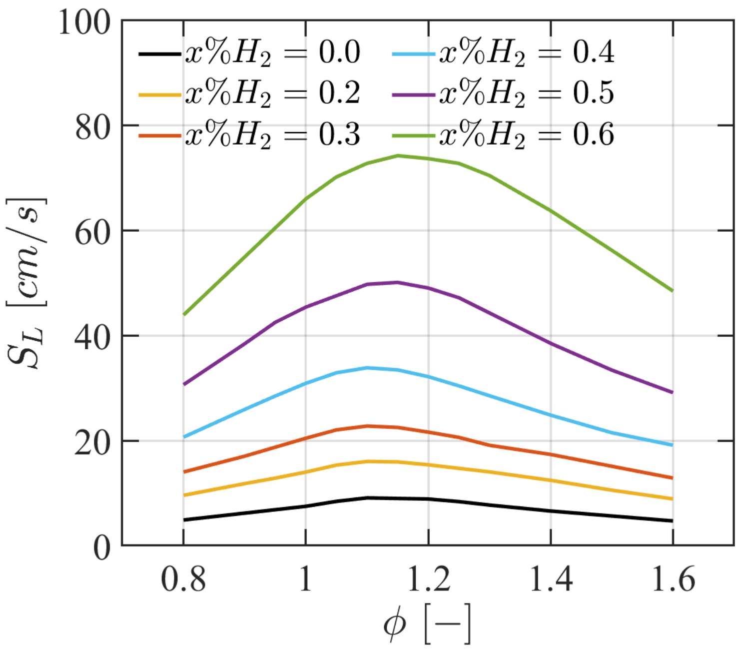
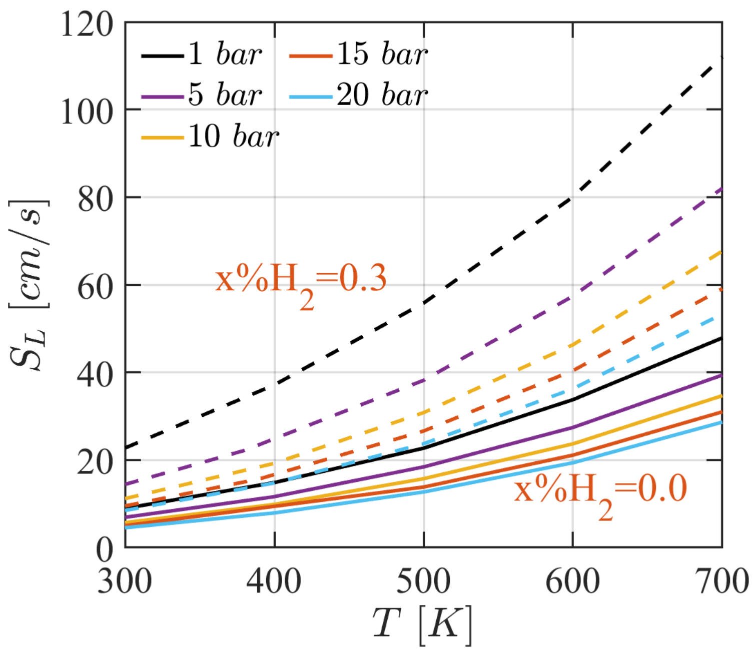
Results – premixed laminar flame speed

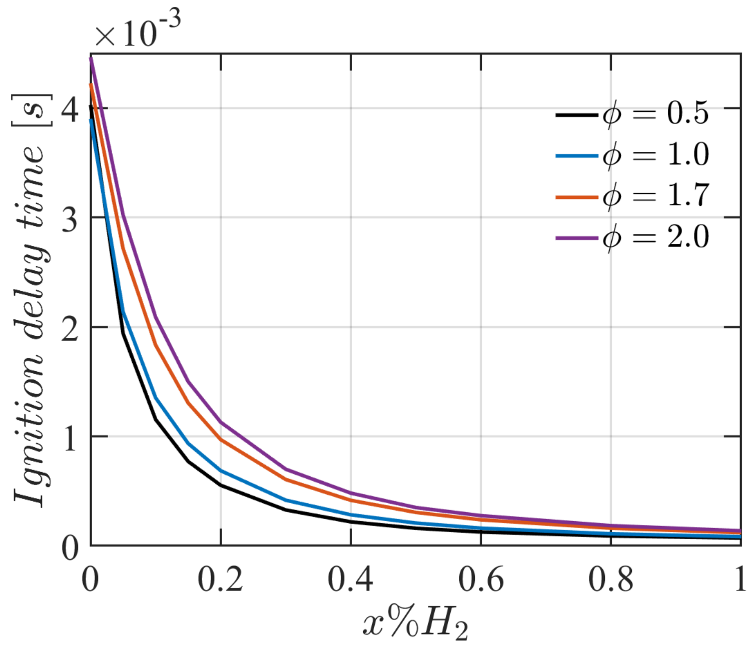
- increases significantly and non-linearly as more hydrogen is introduced
  - Comparable to the flame speed of methane (~37cm/s) as $\phi = 1.1$, x%$H_2 = 0.4$
- peaks when ϕ is around $1.1 - 1.2$
- Increases with the increasing initial temperature and decreases with the increasing initial pressure
  - Less sensitive to initial pressure under high pressure conditions

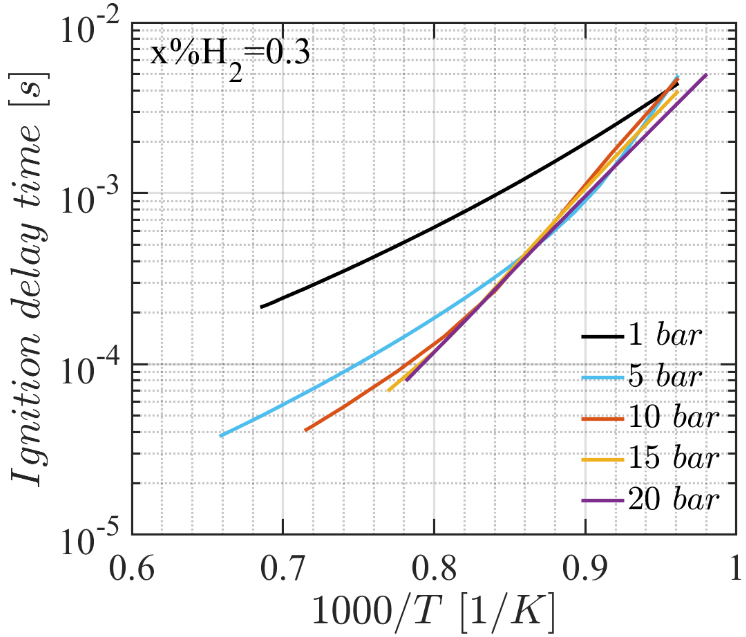




Results – ignition delay

- Shorten considerably with hydrogen addition
  - Minor influence as $x\%H_2$ is over 0.5
- ϕ effect is weaker as more hydrogen addition is added
- A high initial temperature and initial pressure environment promotes ignition
  - Minor influence as the initial pressure is over 10 *bar*

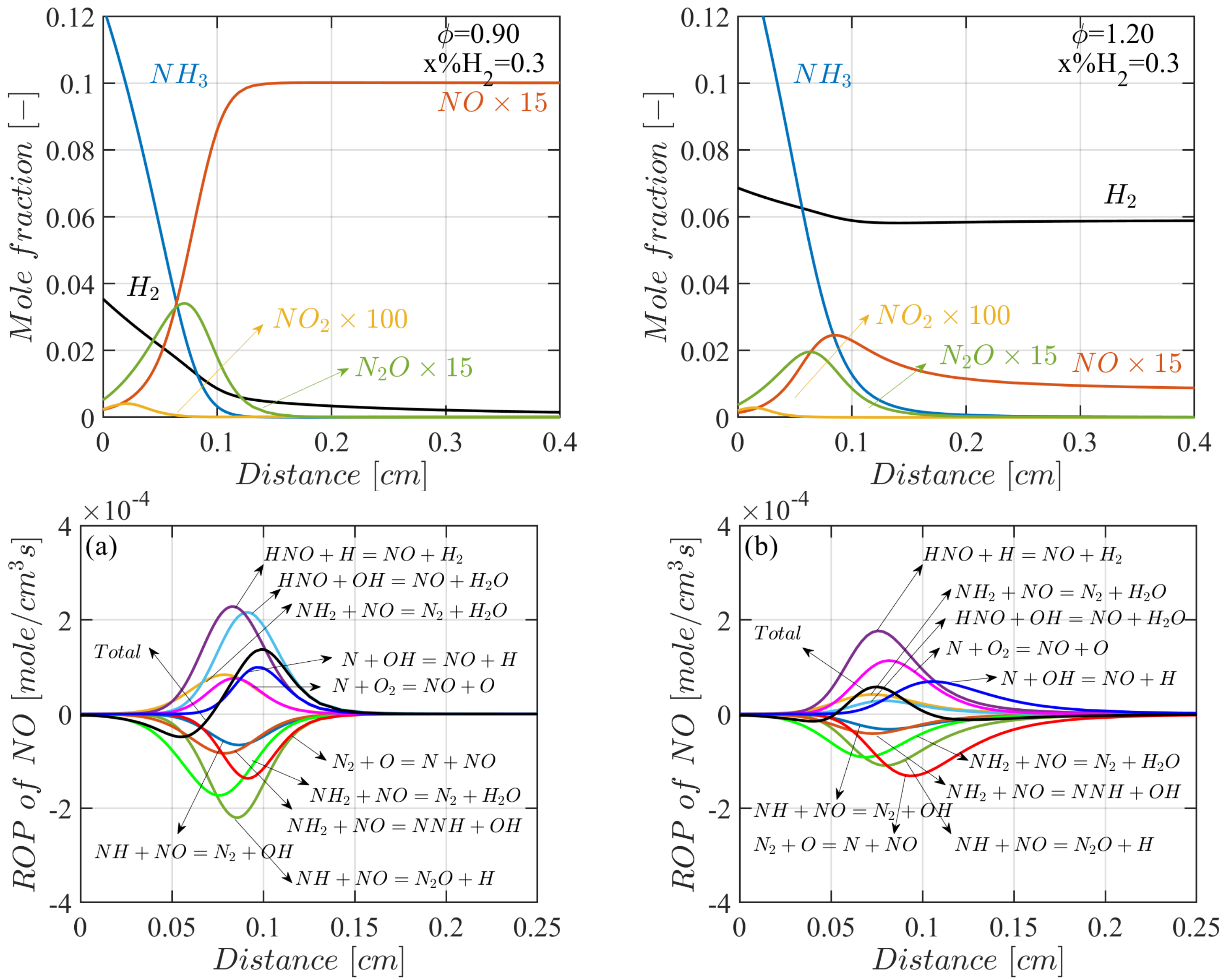




Results – flame species

◆ Equivalence ratio

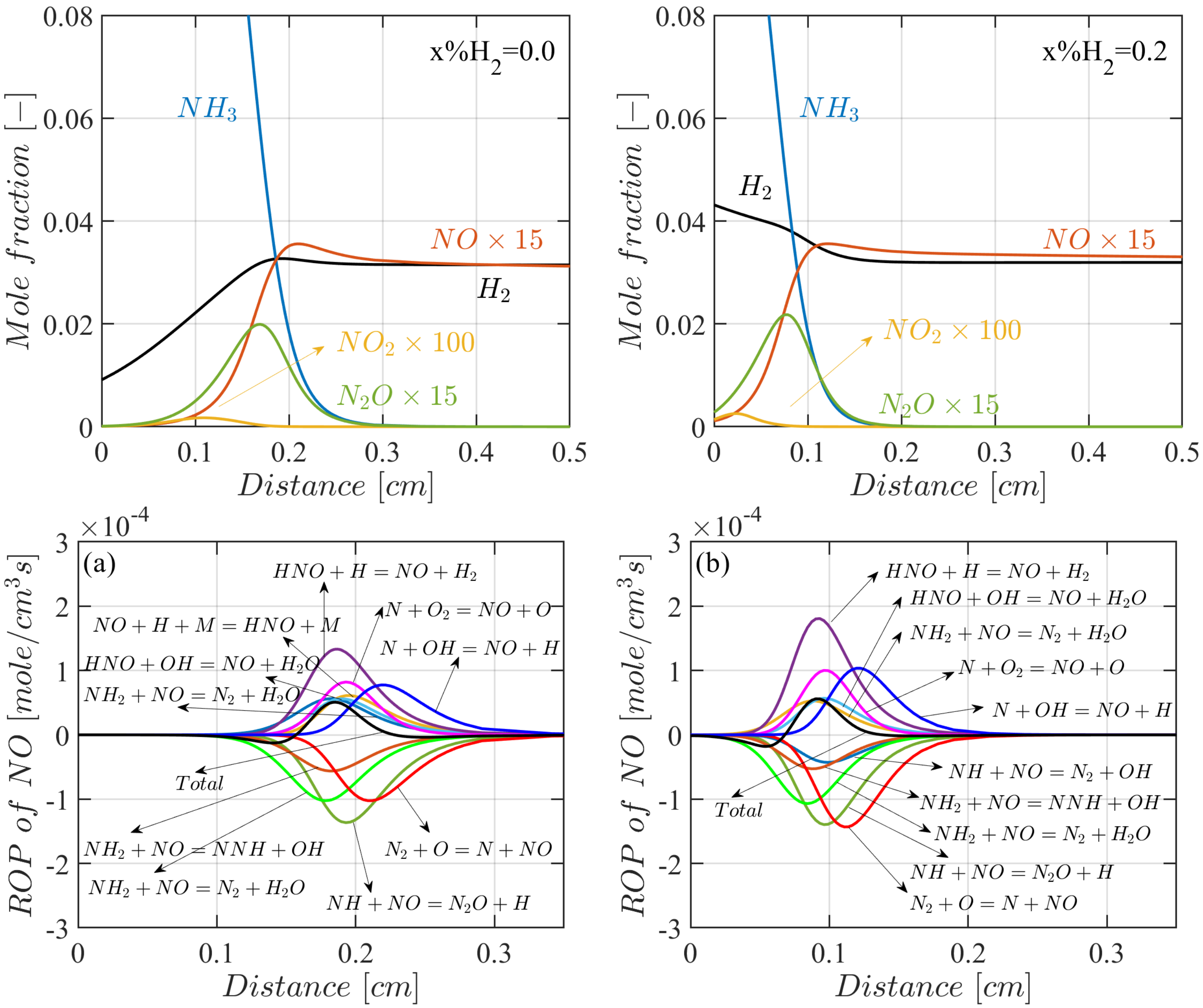
- NO dominates in the NO_x emissions
- With ϕ increases, NO emission is reduced and H_2 is increased apparently
- NO production:
  - $HNO + H/OH$ (fuel-bound NO)
  - $N + O_2/OH$ (thermal NO)
- NO consumption:
  - $NO + NH_i/N$
- In the rich flame, the production of fuel-bound NO decreases and consumption of $NO + N$ reaction increases



Results – flame species

◆ Hydrogen blending ratio

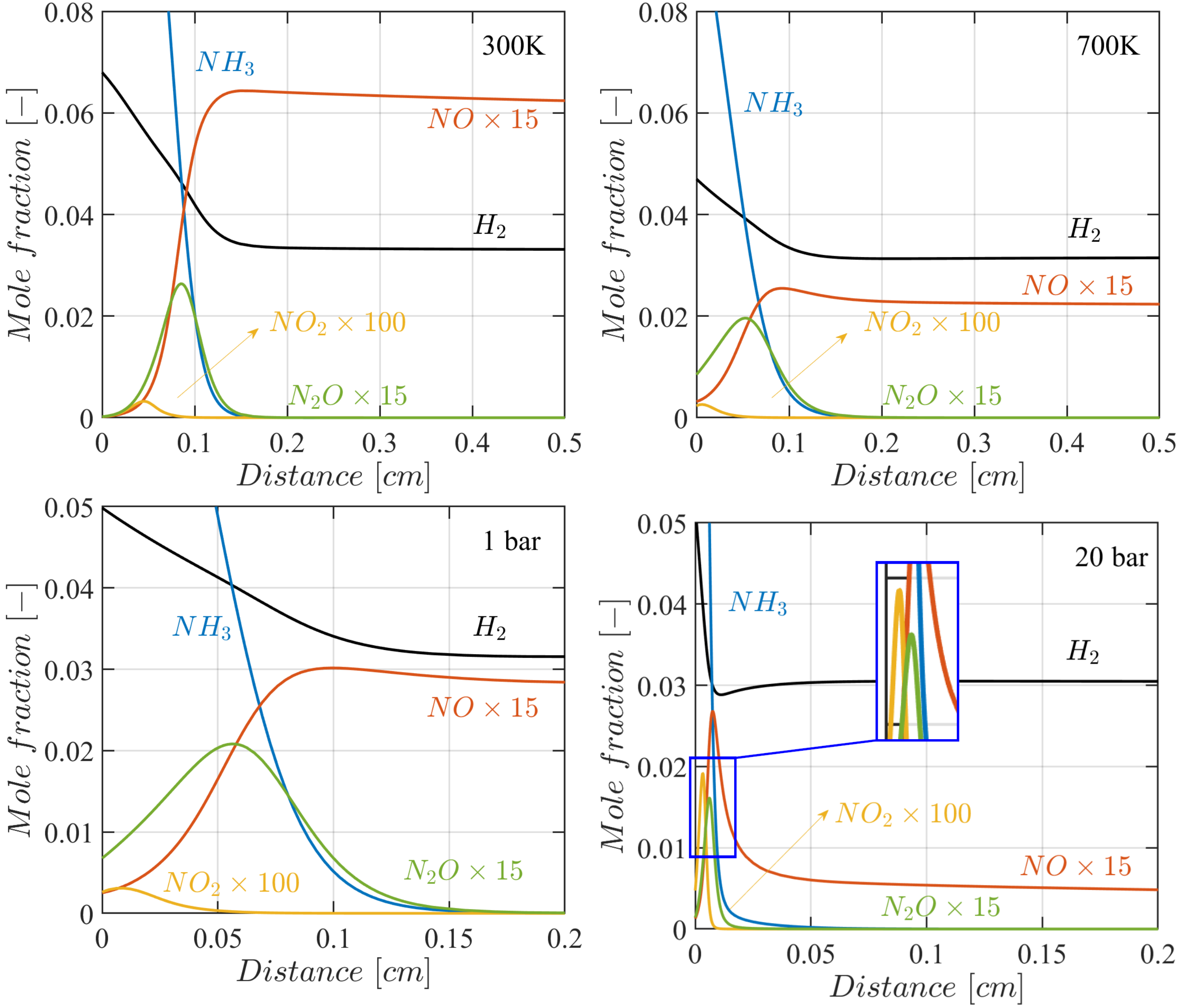
- With $x\%H_2$ increases, NO emission slightly increases and H_2 keeps almost unchanged
- NO emission increases:
  - Thermal NO contribution (production and consumption) increases as $x\%H_2$ increases
- H_2 keeps unchanged:
  - $H_2 + OH$ reaction promotes as $x\%H_2$ increases



Results – flame species

◆ Initial temperature and initial pressure

- NO emission decreases as the initial temperature rises
  - the rate of both production and consumption is decreased
- NO emission also decreases as the initial pressure rises
  - the consumption of NH_i species via the promoted radical combination reactions under high pressure conditions



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  - Flame species
- Summary & conclusions

Summary & conclusions

- Nakamura's mechanism is employed for parametric study.
- An optimized equivalence ratio exists around $1.1 - 1.2$.
- Increasing hydrogen will not cause a large increase in NO emissions at a certain ϕ, while helping to promote the flame speed and ignition.
- High-pressure high-temperature environment is favourable for improving ignition and low NO emission from NH_3/H_2 combustion.

Thank you!