Ammonia for Fuelling Future Energy

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Reduced Chemical Kinetics for CDF Studies of Ammonia-Hydrogen Blends in Gas Turbine Swirl Combustors

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1 Introduction

Chemical storage of energy can be considered via hydrogen or carbon-neutral hydrogen derivatives. Ammonia is one such example. Similar to synthesized hydrogen, ammonia is a product that can be obtained either from fossil fuels, biomass or other renewable sources. Some advantages of ammonia are its low cost per unit of stored energy, relatively high volumetric energy density, maturity of handling and distribution practice, and good commercial viability. Ammonia recovered by harvesting of renewable electricity sources is carbon-free yielding no direct greenhouse gases. However, a viable energy system based on ammonia faces four primary barriers:

1. High-efficiency, carbon-free synthesis.

2. High-efficiency, low emission, power generation from small to utility-scale units.

3. Public acceptance, safety regulations and appropriate community engagement.

4. Economic viability for full global deployment compared to other technologies.

It is important to emphasize that ammonia is complementary to the delivery of the "Hydrogen Economy", as ammonia is hydrogenated nitrogen. Hence, the "Ammonia community" is part of the "Hydrogen community".

2 Aims

- ✓ Employ CFD simulation using new reduced chemical kinetic models (Glarborg et al, 2018) to assess their suitability for numerical combustion studies;
- ✓ Explore the use of these models for design of new injection strategies for ammonia based blends;
- ✓ Correlate numerical calculations to experimental findings for model improvement and combustor design development.

3 Setup

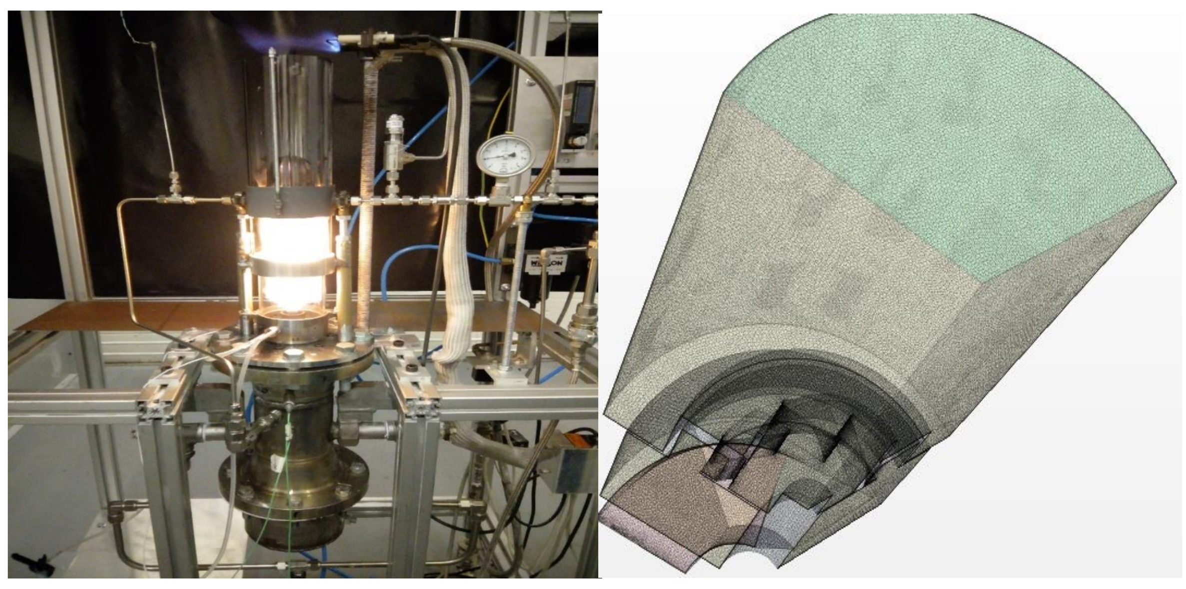

Figure 1. A 20kW Swirl Burner (left) used for FTF analyses has been modelled (right) for this project.

- ✓ A double precision CFD simulation was done by STAR-CCM+.
- ✓ A 1.6 Million cells mesh was employed, thus requiring HPC facilities for resolution.
- ✓ Inlet conditions were 300K and atmospheric pressure, with an inlet velocity of 3m/s.
- ✓ A 70-30% (mol%) blend NH3-H2 was used as in previous experiments performed somewhere else (Valera-Medina et al 2019)
- ✓ RANS K-W SST with resolution of Glarborg's reduced mechanism was employed.

4 Reduced Reaction Model

- ✓ Detailed reaction model: Glarborg model (151-species, 1397-reaction)
- ✓ Reduction target conditions: Φ = 0.5~2.0, P = 1atm~50atm}, and T = 1000K~2000K
- ✓ Reduction method: DRGEP. Program: ReaxRed.
- ✓ Finally, skeletal mechanism containing 27-species and 190-reactions is obtained.

Method	Name	Species, Reactions	Max. error, %					Average. error, %			
			20%NH3	50%NH3	80%NH3	100%NH3		20%NH3	50%NH3	80%NH3	100%
DRGEP	GR1_AM	68S, 690R	0.267	0.151	0.307	0.430		0.0168	0.0131	0.0364	0.0741
Remove C-Species	GR_AH	27S, 190R	0.267	0.151	0.306	0.430		0.0164	0.0131	0.0365	0.0741

Table 1. Reduced kinetic mechanisms for NH_3+H_2 combustion

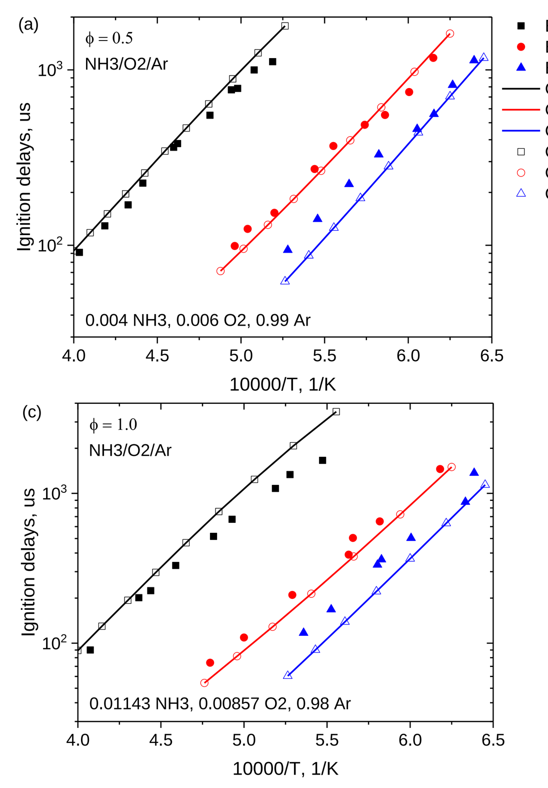

Figure 2. Ignition delay times for NH_3 + O_2 + Ar mixtures at different pressures with detailed and reduced models. The source of experimental data: Mathieu et al. The ignition delay times are modeling with $(d[OH]/dt)^{max}$

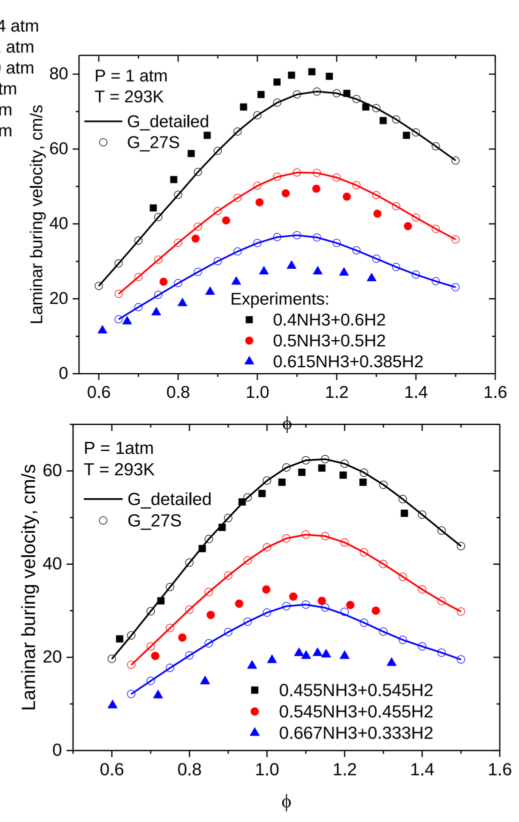

Figure 3. Laminar burning velocity of NH_3+H2/air flames at the temperature of 293K and pressure of 1 atm for various equivalence ratios. The source of experimental data: Li et al.

5 CFD Results & Validation

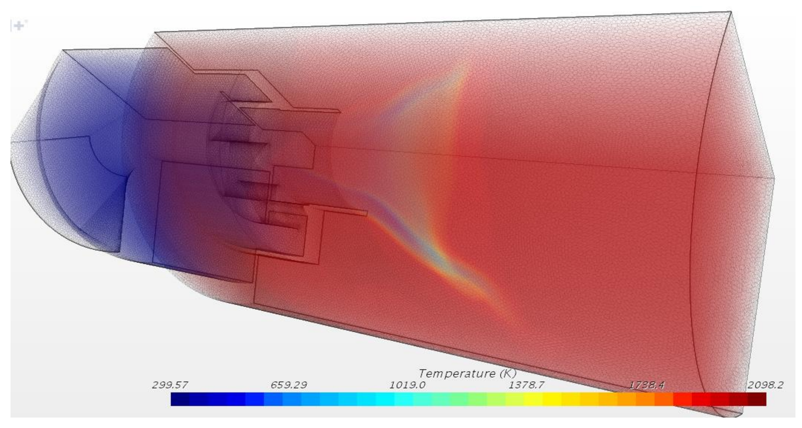

Figure 4. Volumetric temperature profile. Units [K]

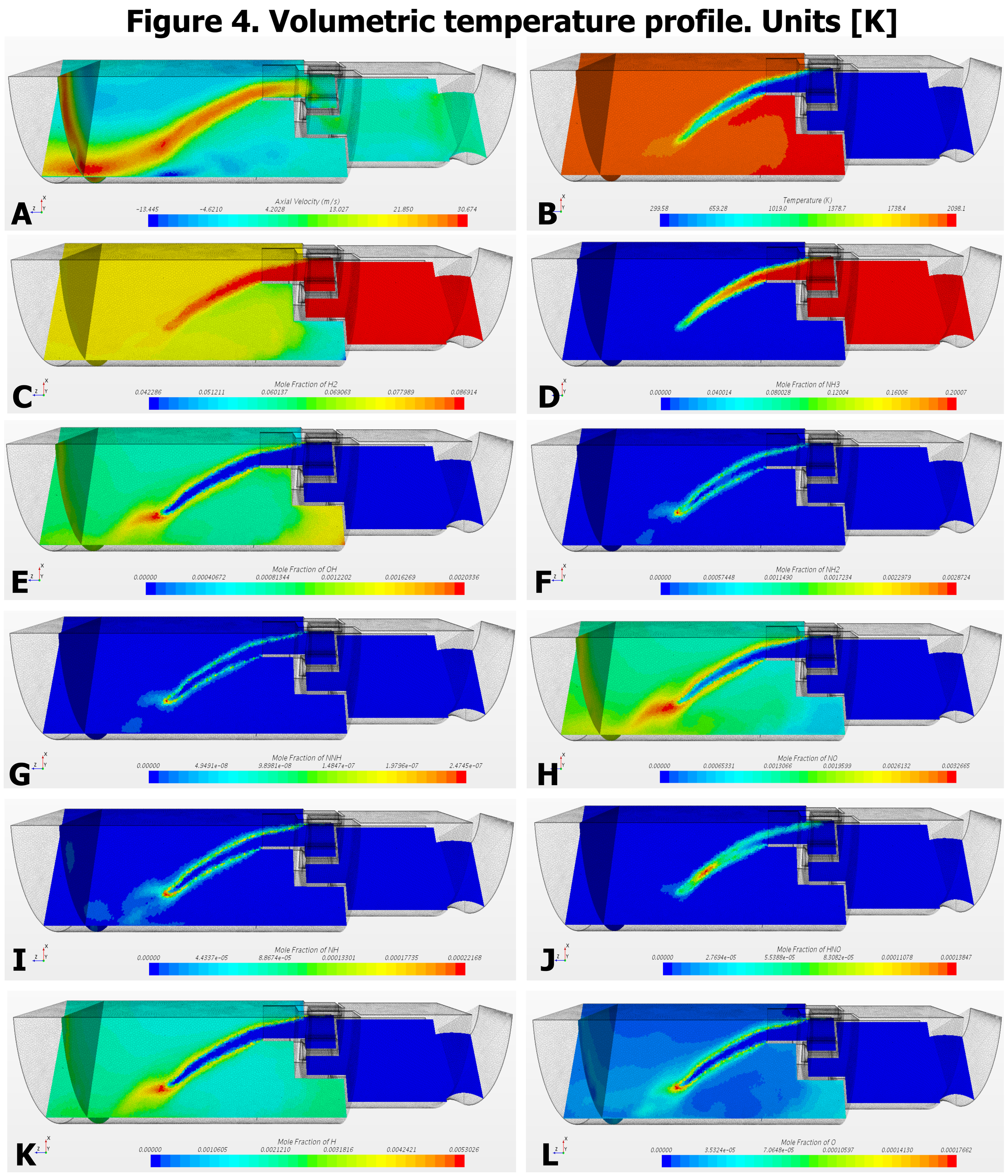

Figure 5. Results obtained from numerical campaign using 27 species. A) Axial velocity [m/s]; B) Temperature [K]; C) H2 molar frac.; D) NH3 molar frac.; E) OH molar frac.; F) NH2 molar frac.; G) NNH molar frac.; H) NO molar frac.; I) NH molar frac.; J) HNO molar frac.; K) H molar frac.; L) O molar frac.

6 DISCUSSION

- ✓ Results show the high production of hydrogen post-flame. These results are in accordance with experimental tests (Pugh et al, 2018).
- ✓ However, some reactions seem to fast (i.e. NH3 dissociation) whilst hydrogen reactivity is not as high, thus showing patterns of complete ammonia consumption with high remnant of hydrogen gas.
- ✓ NO seems to be produced essentially at the flame front (as expected) and in regions of high recirculation, suggesting the study of these zones for De-Noxing strategies.
- ✓ NO is also linked to the production of NH and H, as described somewhere else (Glarborg et al, 2018).
- ✓ Further studies are required with other reduced mechanisms, i.e. more species.

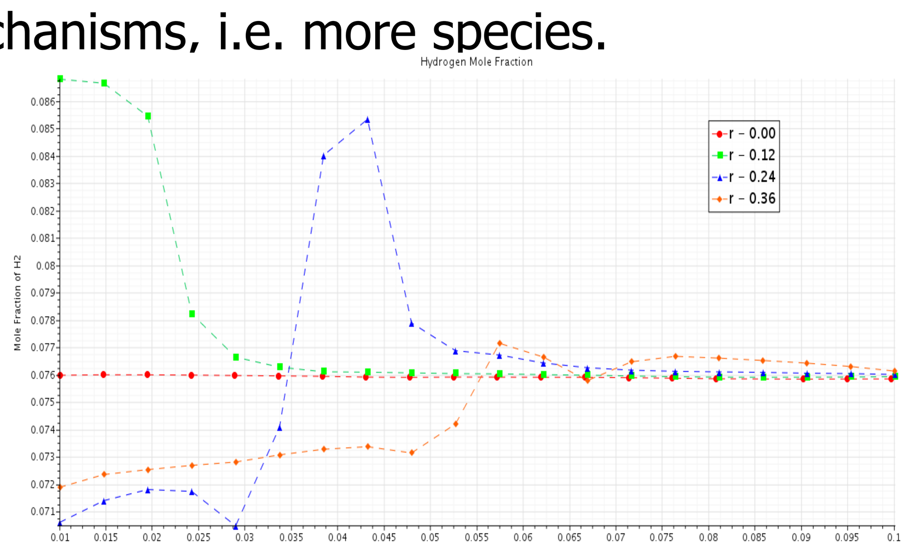

Figure 6. Hydrogen is consumed at the flame, although the molecule is also produced by ammonia dissociation.

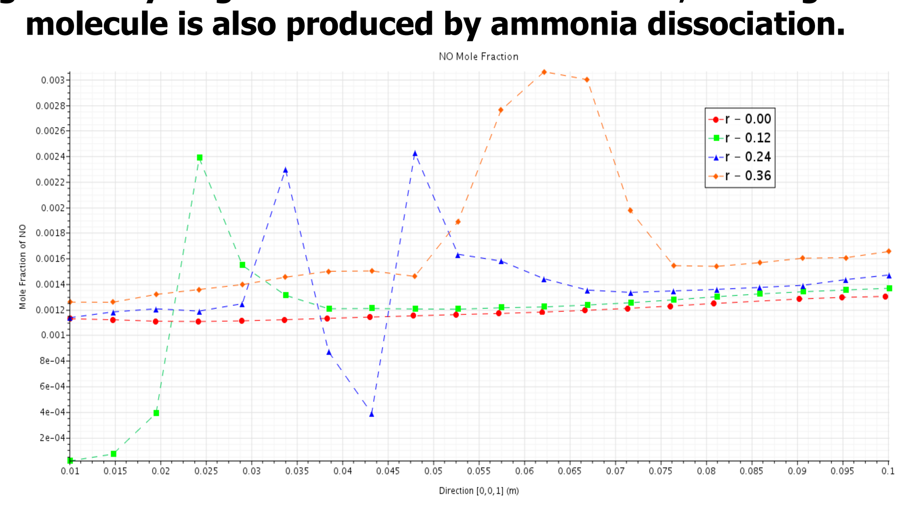

Figure 7. NO production, with peaks across the flame front and in recirculation zones.

7 Conclusions

- ✓ CDF modelling employing reduced mechanisms can allow full characterisation of species difficult to track experimentally.
- ✓ However, current models still need to be tested using ammonia blends that are potential candidates for power generation.
- ✓ Results from these trials suggest that these models, although relevant to most findings and current knowledge on ammonia reactivity, require further development to properly characterise a complex swirl combustion system.
- ✓ Further works will be pursued to analyse reactions with more species, complemented with experimental tests for validations purposes and future combustion designs.

8 References

O. Mathieu, E.L. Petersen, Experimental and modeling study on the high-temperature oxidation of Ammonia and related NOx chemistry, Combustion and Flame 162 (2015) 554–570.

Li J, Huang H, Kobayashi N, He Z, Nagai Y. Study on using hydrogen and ammonia as fuels: Combustion characteristics and NOx formation: hydrogen and ammonia as fuels. Int J Energy Res 2014;38(9):1214–1223.

Glarborg P, Miller JA, Ruscic B, Klippenstein SJ. Modeling nitrogen chemistry in combustion. Prog. Energy Combust Sci 2018b;67:31-68.

Pugh D, Bowen P, Valera-Medina A, Giles A, Runyon J, Marsh R. Influence of steam addition and elevated ambient conditions on NO x reduction in a staged premixed swirling NH 3 /H 2 flame. Proc Combust Inst 2019. 37; 5401-5409

Valera-Medina A, Gutesa M, Xiao H, Pugh D, Giles A, Goktepe B, Marsh R, Bowen P. Premixed ammonia/hydrogen swirl combustion under rich fuel conditions for gas turbines operation, Int J Hydro Energy 2019, 44; 8615-8626.