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Numerical Simulation using Ammonia/Methane blends in a Swirl Gas Turbine Combustor

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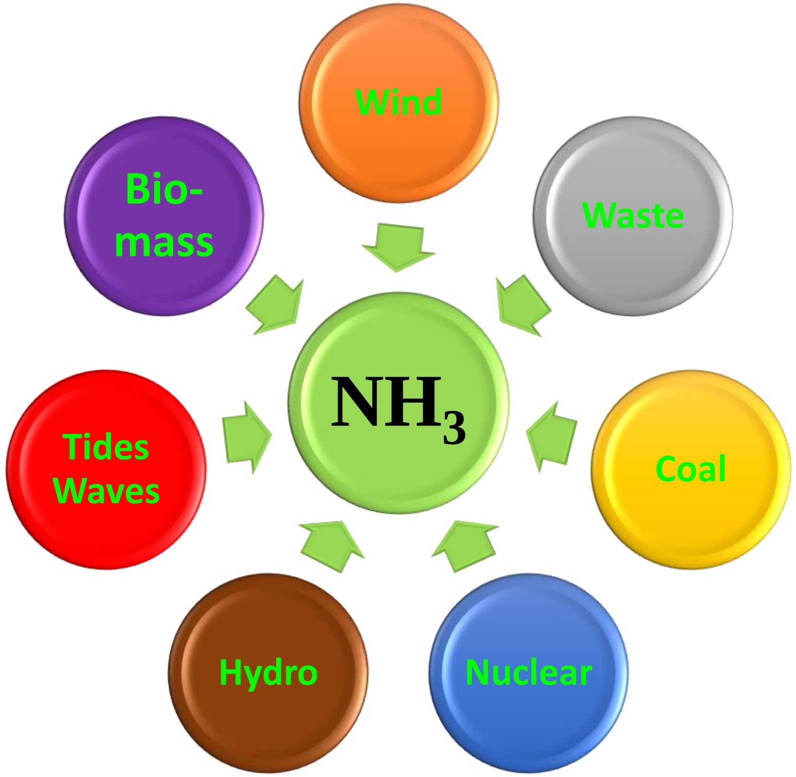
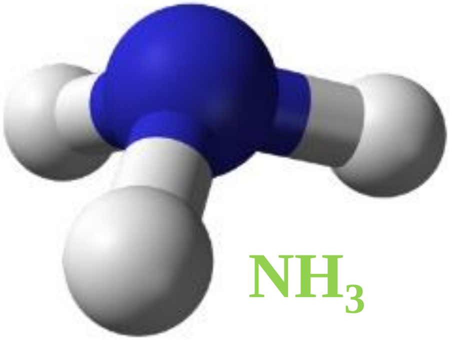
SCHOOL OF ENGINEERING

1. Ammonia as a Sustainable Fuel

- Carbon-free fuel
- High hydrogen density
- Combustion process:
  $NH_3+O_2=N_2+H_2O$
- Easy to store, transport
- A high octane rate of 110 –130





NH_3

- Poisonous
- Corrosive
- Fuel bond NOx emissions
- Narrow flammability range

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Ammonia as a Sustainable Fuel

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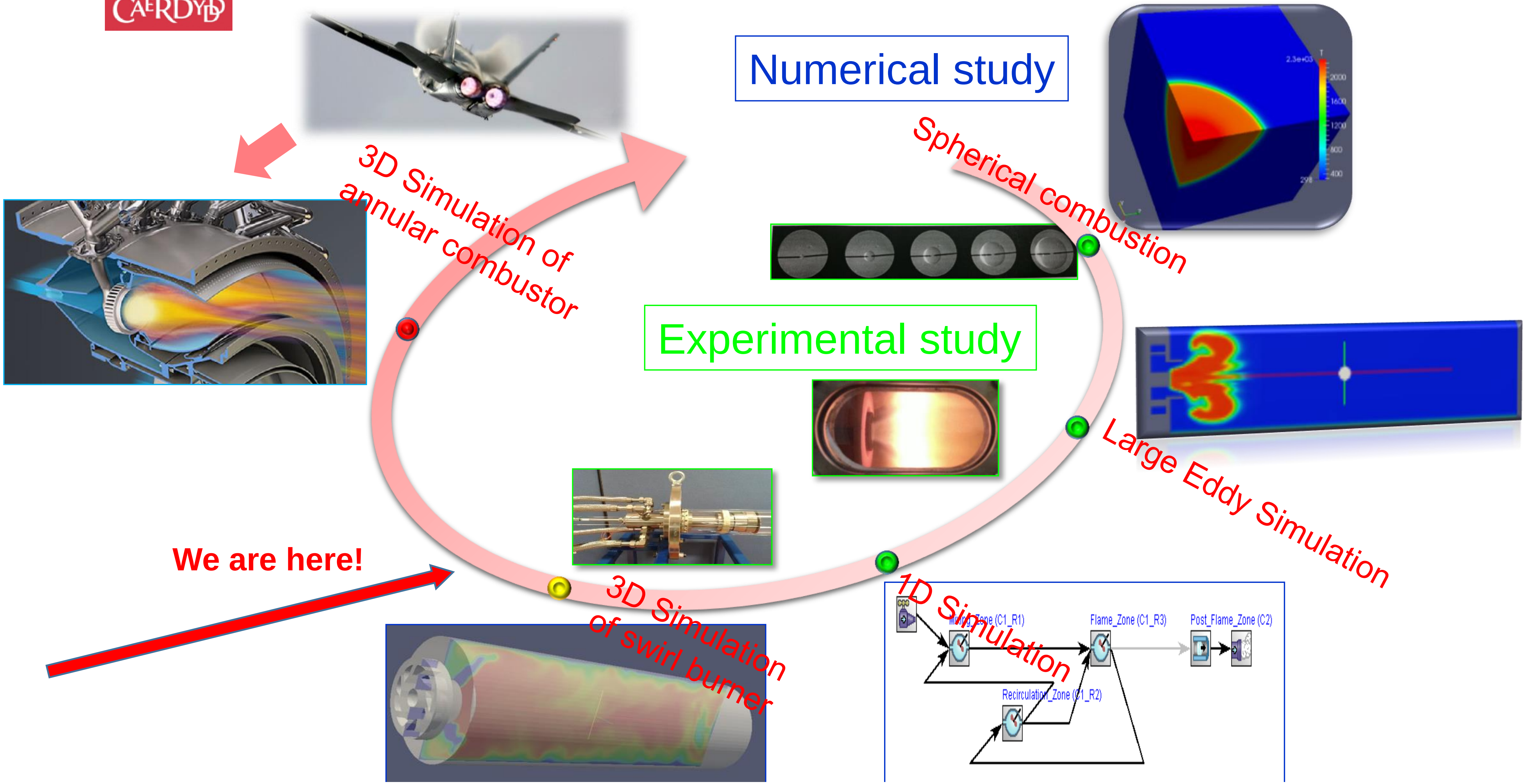
2. Research Plan



3. Large Eddy Simulation

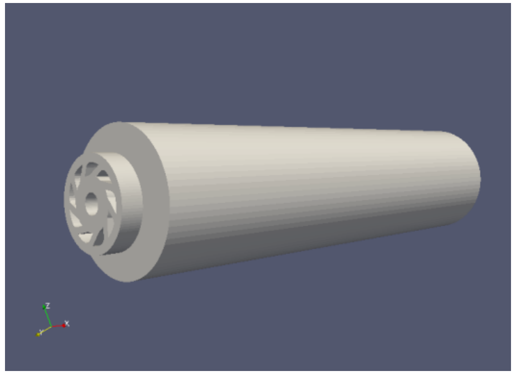


Fig.1. Combustor configuration

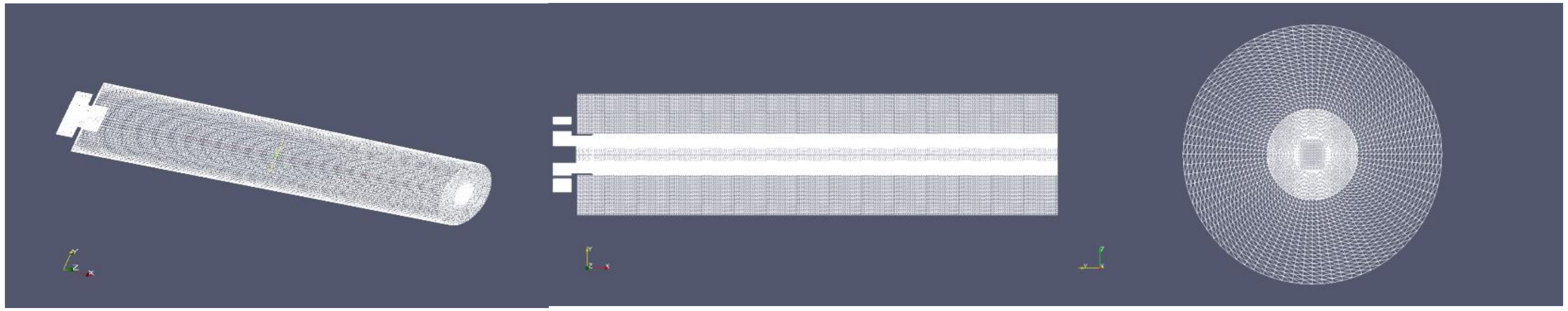


Fig.2. Mesh of the combustor

Structured Mesh of 0.9 million cells

3D Large Eddy Simulation

Operating pressure		2bar
Oxidiser (mol%)	O_2	21%
	N_2	79%
Fuel (mol%)	CH_4	38%
	NH_3	62%
Mass flow		10.5g/s
Inlet Temperature		300K
Wall condition		Isothermal

Table1. Boundary conditions of combustor model

Platform: OpenFOAM
Turbulence: Smagorinsky model
Reaction: Konnov’s Mechanism
Combustion: Partially Stirred Reactor (PaSR)

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Detailed Chemical Kinetics Mechanisms

Global Mechanism:

$NH_3+O_2=N_2+H_2O$

Detailed Mechanism:

e.g. KONNOV's Mechanism (1410 reactions & 94 species)

```
NH3+O=NH2+OH          NH+NH=N2+H2                      NO+HCO=CO+HNO
NH3+OH=NH2+H2O        NH2+M=NH+H+M                     NO2+CO=CO2+NO
NH3+HO2=NH2+H2O2      NH+H2=NH2+H                      NO2+HCO=H+CO2+NO
NH2+HO2=NH3+O2        NH2+N=N2+H+H                     CH3O+NO2=HONO+CH2O
NH2+O=H2+NO           NH2+NH=N2H2+H    ......  ......  CH3O+NO=CH2O+HNO
NH2+O=HNO+H           NH2+NH=NH3+N                     NO2+CH2O=HONO+HCO
NH2+O=NH+OH           NH3+NH=NH2+NH2                   NO+CH2O=HNO+HCO
NH2+OH=NH+H2O         NH2+NH2=N2H2+H2                  NO2+HCO=HONO+CO
NH2+OH=NH2OH          N2H3+H=NH2+NH2                   NO2+HCO=OH+NO+CO
NH2+HO2=HNO+H2O       NH3+M=NH2+H+M                    NCO+N=NO+CN
                                                       END
```

3D Simulation Results

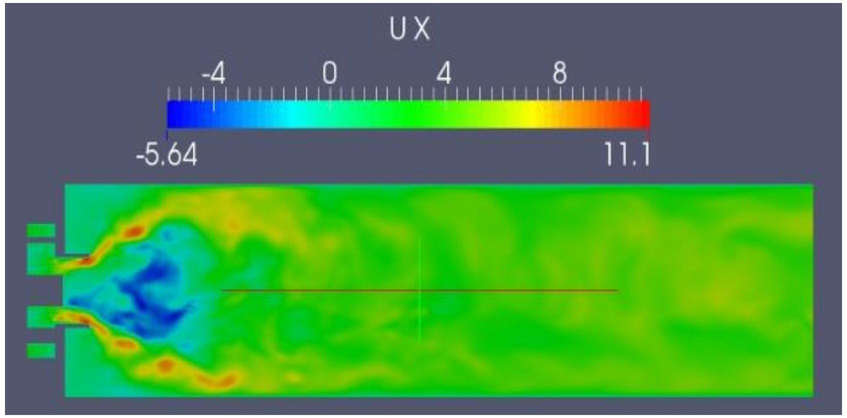

Fig.3. Velocity distribution in the swirl burner

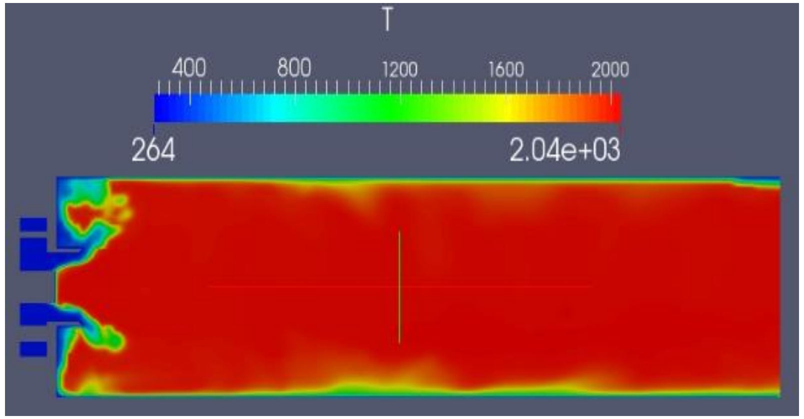

Fig.4. Temperature field, in K

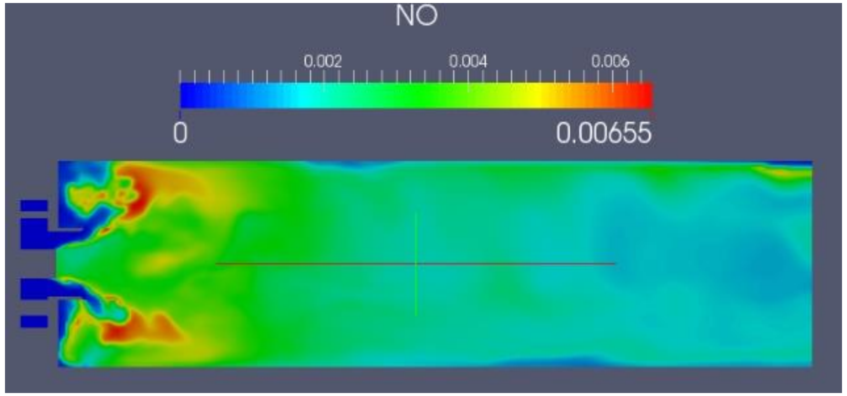

Fig.4. NO distribution across the burner

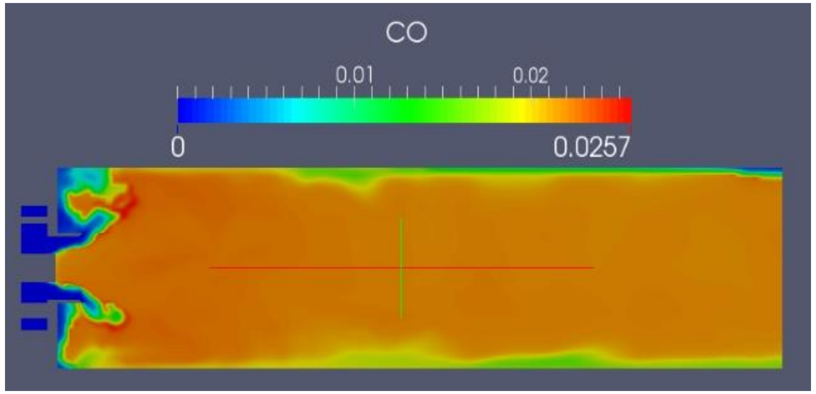

Fig.5. Carbon monoxide concentration

3D LES Simulation Results

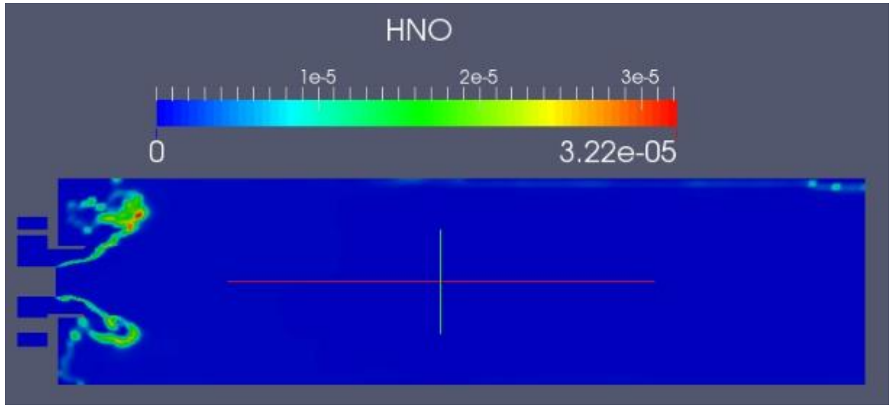

Fig.6. HNO distribution across the burner

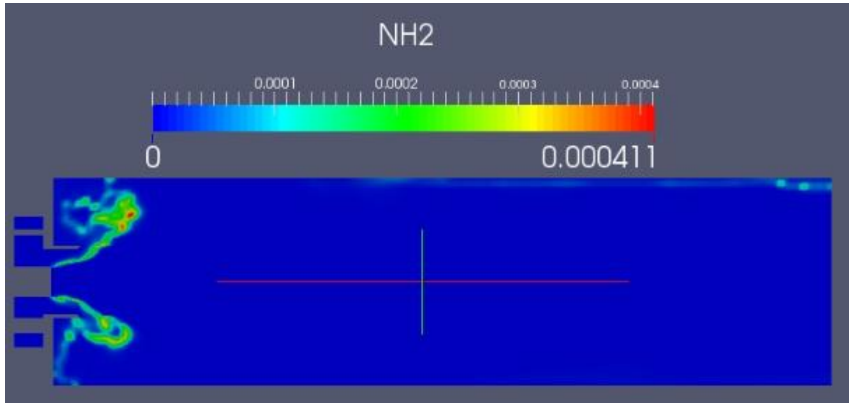

Fig.7. NH2 distribution across the burner

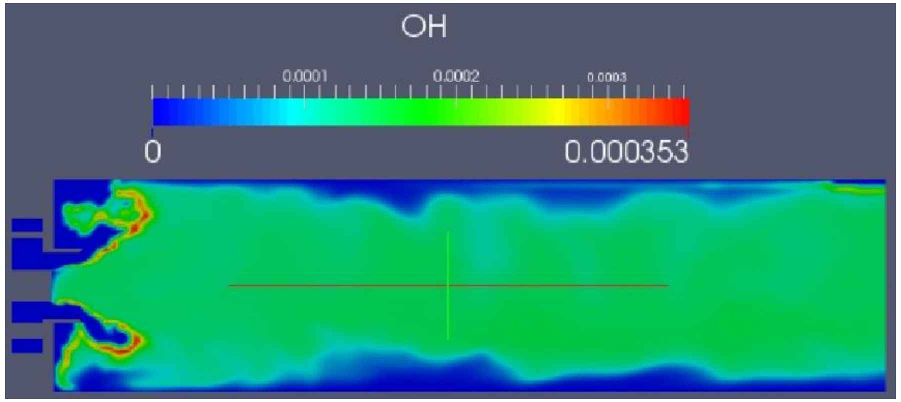

Fig.8. OH distribution across the burner

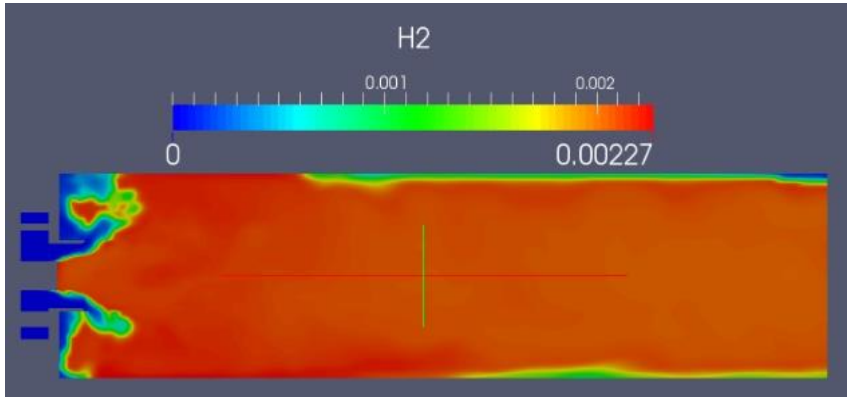

Fig.9. Hydrogen concentration

3D LES Simulation Results

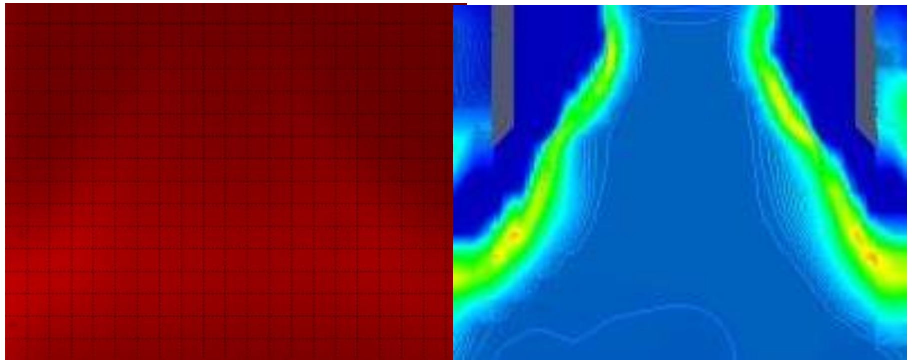

Fig.10. OH distribution in the flame
(left-experiment, right-simulation)

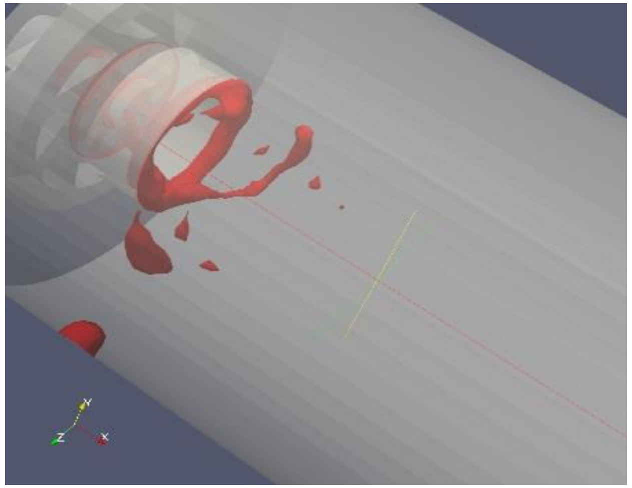

Fig.11. Iso-surface of pressure

4. Chemical Reactor Network

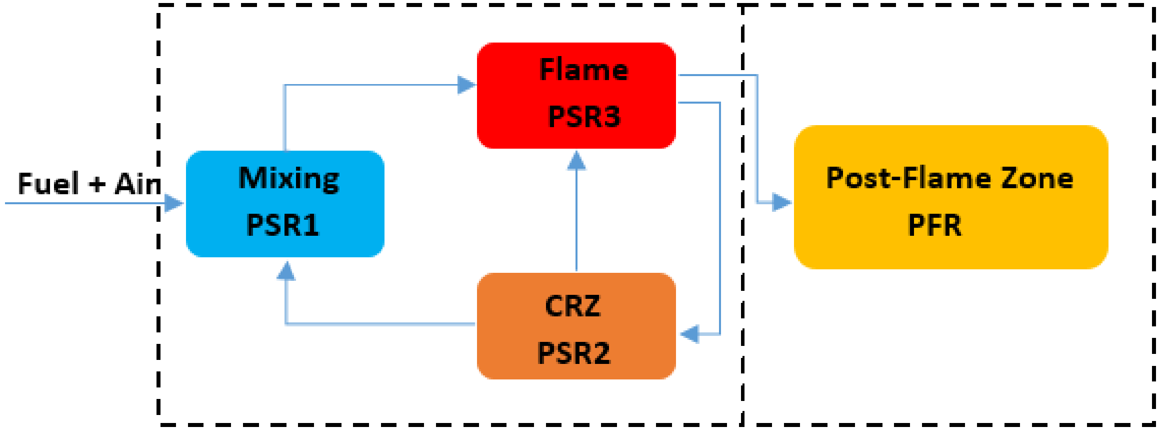

Fig.12. Chemical Reactor Network (CRN)

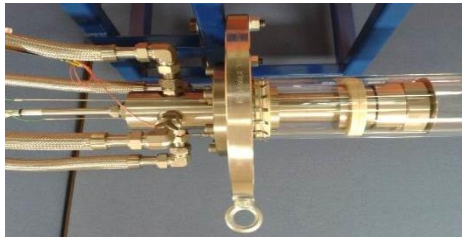

Fig.13. Gas Turbine Combustor at the GTRC

Gas Turbine Network

CRN Simulation Results

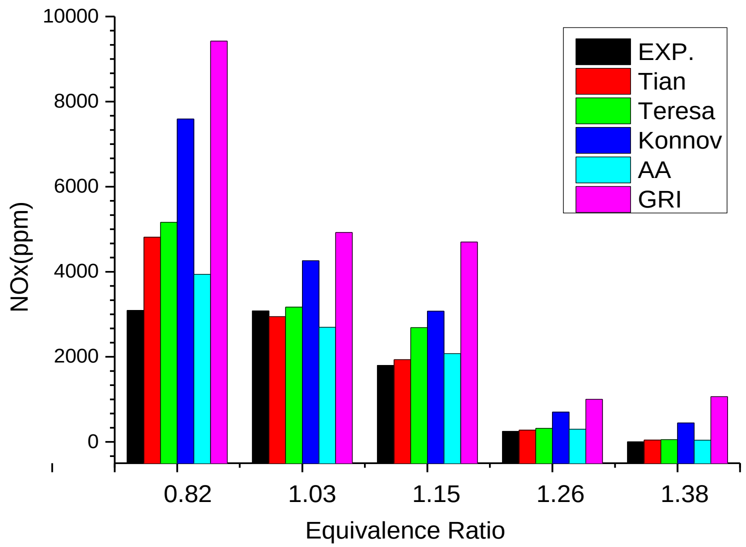

Fig.14. NOx prediction by different mechanisms (1 atm)

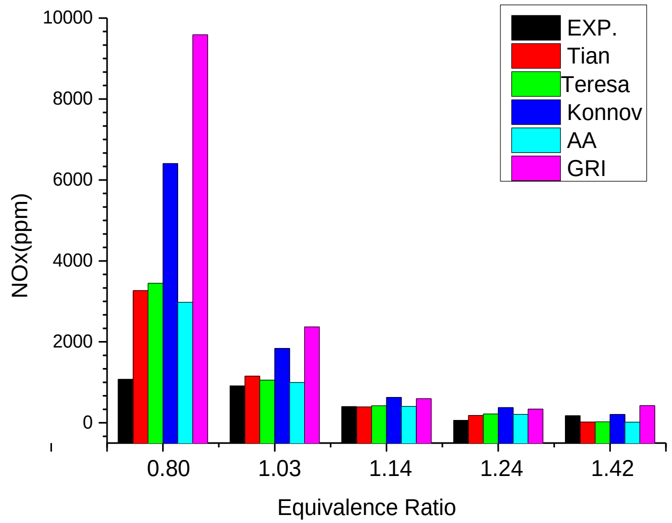

Fig.15. NOx emission as at 2atm

Ammonia combustion mechanisms :
Konnov's, Tian's, Teresa's, AA's mechanism and GRI 3.0 mechanism.

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1D Simulation Results

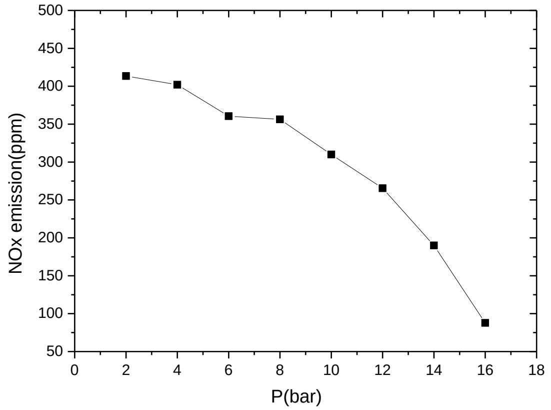

Fig.16. NOx emission as at different pressure

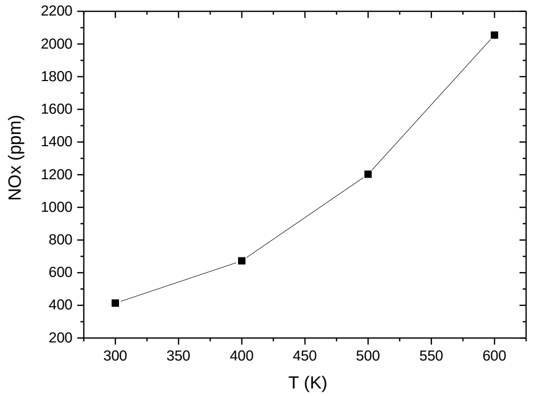

Fig.17. NOx emission as at different inlet temperature

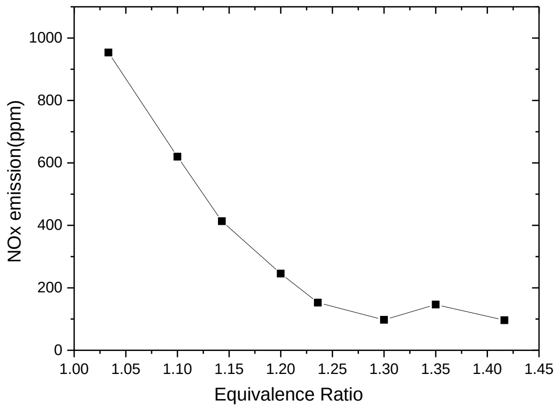

Fig.18. NOx emission as at different E.R.

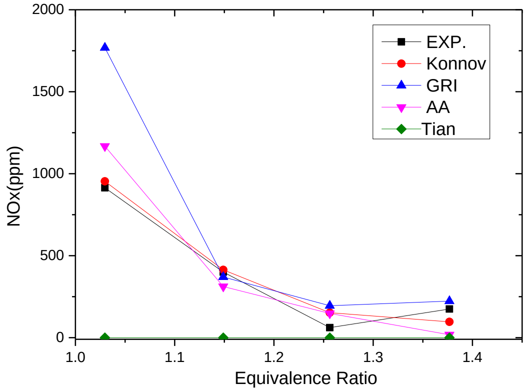

Fig.19. NOx prediction by different chemical mechanisms

1D Simulation Results

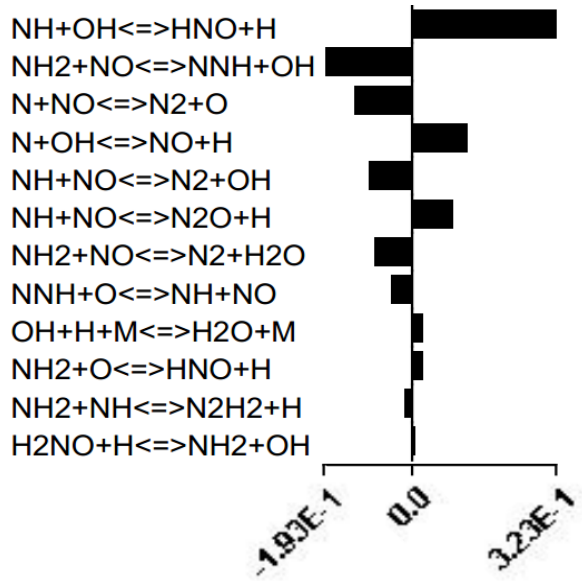

Fig.20. NO sensitivity under 17 atm, E.R.=1.14

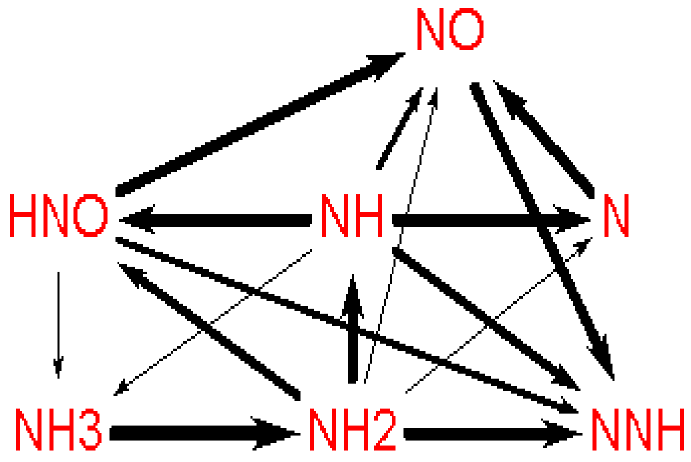

Fig.21. Pathway analysis of the NO formation in the flame zone

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5. Future Work

- More ***accurate models*** for ammonia/methane will be developed to explore the good potential for power generation.
- More experimental and numerical studies will be conducted on a more ***advanced annular combustor*** to get a better combustion performance of ammonia.
- Cooperation with Limerick university will help develop ***new detailed chemical mechanisms*** particularly for ammonia combustion under the real gas turbine operation conditions.
- Ammonia with ***other green fuels*** like hydrogen will be investigated to enhance the combustion performance.

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