Evaluation of Minimum NO_x Emission from Ammonia Combustion

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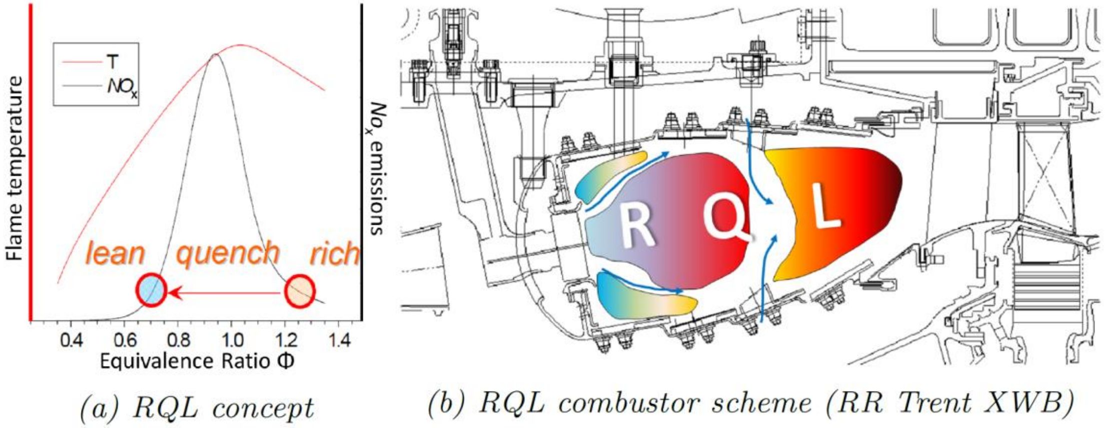
Introduction

- Ammonia is a potential carbon-free fuel
- Increased NO_x concern with fuel-bound nitrogen
- This work explores staged combustion for low NOx
- Rich-Quench-Lean (RQL) used in systems with high turndown (aviation) is promising for ammonia
    - Previous studies[1] observed emissions as low as 50 ppm NO_x emissions
    - Previous studies[1] showed large amounts of H_2 produced in rich ammonia flames (over 3000 ppm)



(a) RQL concept *(b) RQL combustor scheme (RR Trent XWB)*

Innocenti, A., 2016. Numerical analysis of the dynamic response of practical gaseous and liquid fuelled flames for heavy-duty and aero-engine gas turbines.

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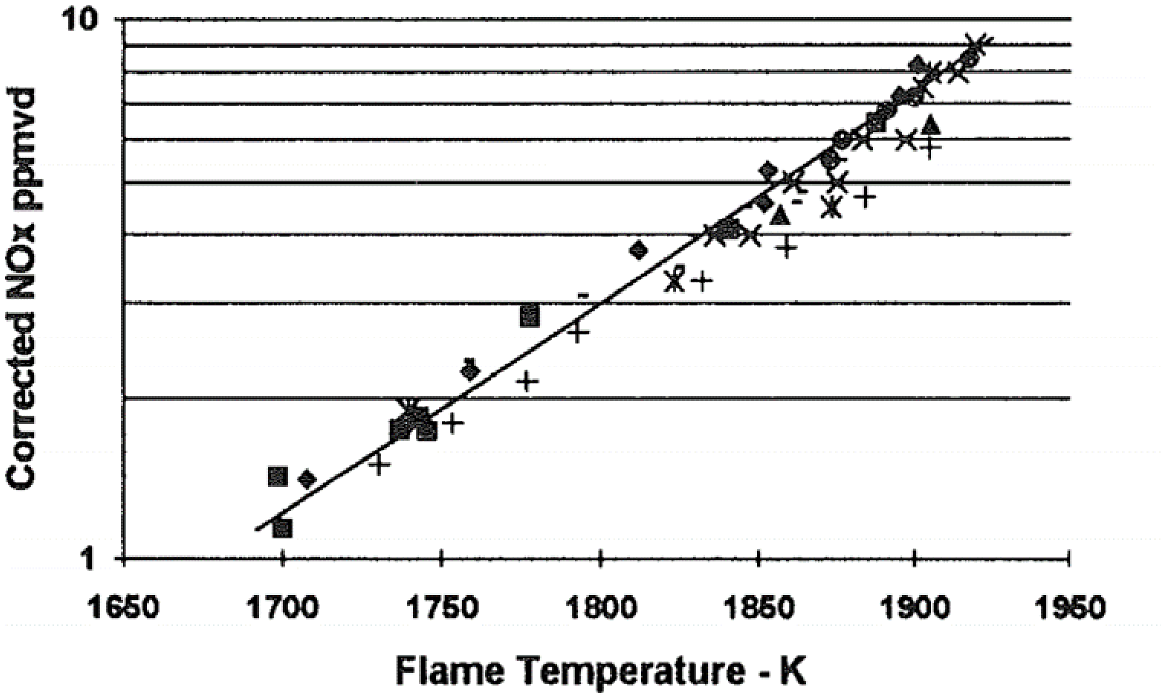
[1] R.C. Rocha, M. Costa, X.-S. Bai, Combustion and Emission Characteristics of Ammonia under Conditions Relevant to Modern Gas Turbines, Combustion Science and Technology 193 (2021) 2514-2533.

Motivation

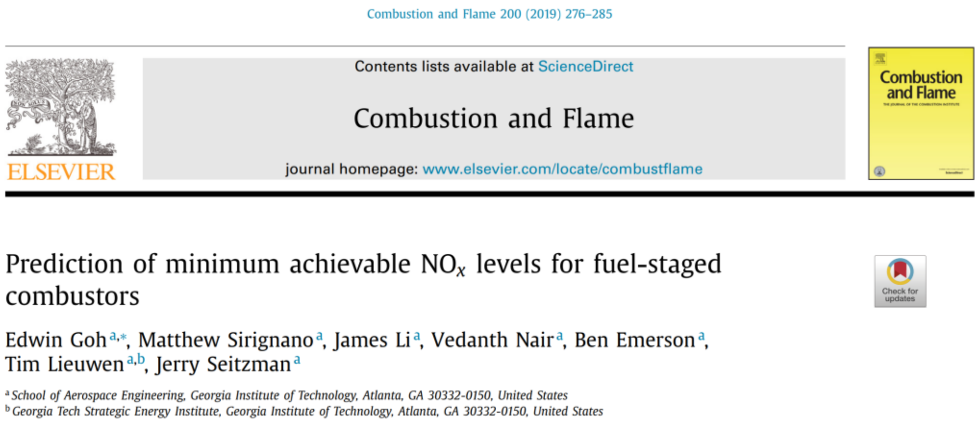
- **Research Question:** what is the theoretical minimum possible NO_x emission from ammonia combustion?
  - Not simulating a specific combustor
  - Addressing what is possible with technological development
  - “NOx entitlement” for ammonia RQL
- Minimization problem applied to RQL architecture
  - Vary combustor parameters
  - Minimize NO_x low while limiting H_2 emissions
- Analyze sensitivities to firing temperature, combustor pressure, global residence time, and RQL parameters



NOx entitlement for lean premixed natural gas. Reproduced from Leonard, G. and Stegmaier, J., 1994. Development of an aeroderivative gas turbine dry low emissions combustion system.

Approach

- Revisiting previous staged combustor NOx entitlement modeling of Goh et al.
- Modeled using reactor network model in Cantera
- Each stage represented as 1-D flame with perfect mixing assumption
- Perfect mixer is an adiabatic, nonreacting constant pressure batch reactor



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Prediction of minimum achievable NO$_x$ levels for fuel-staged combustors

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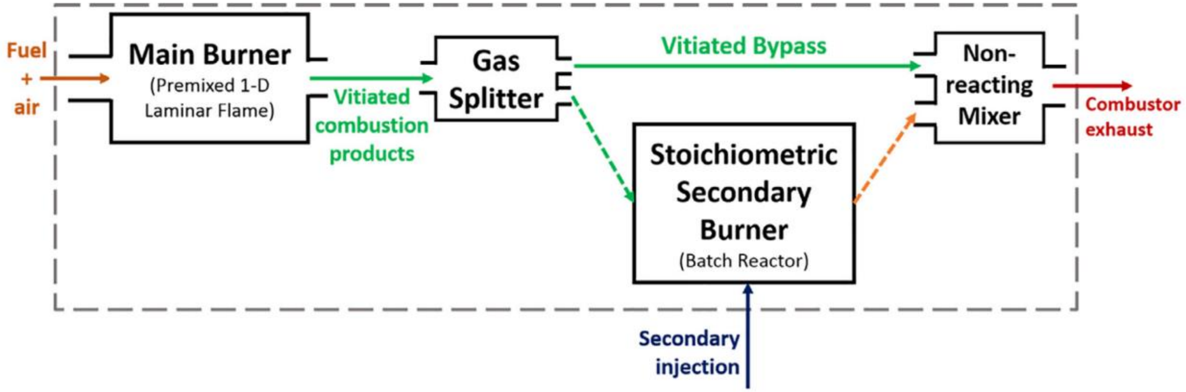
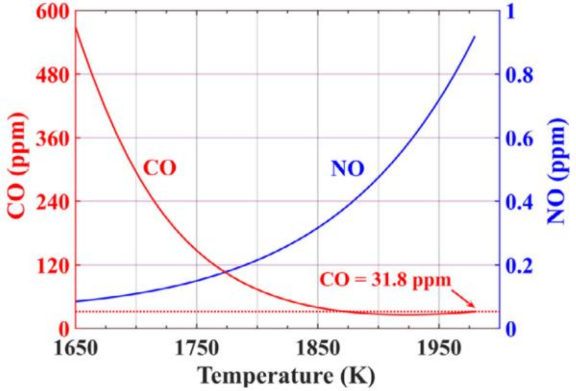
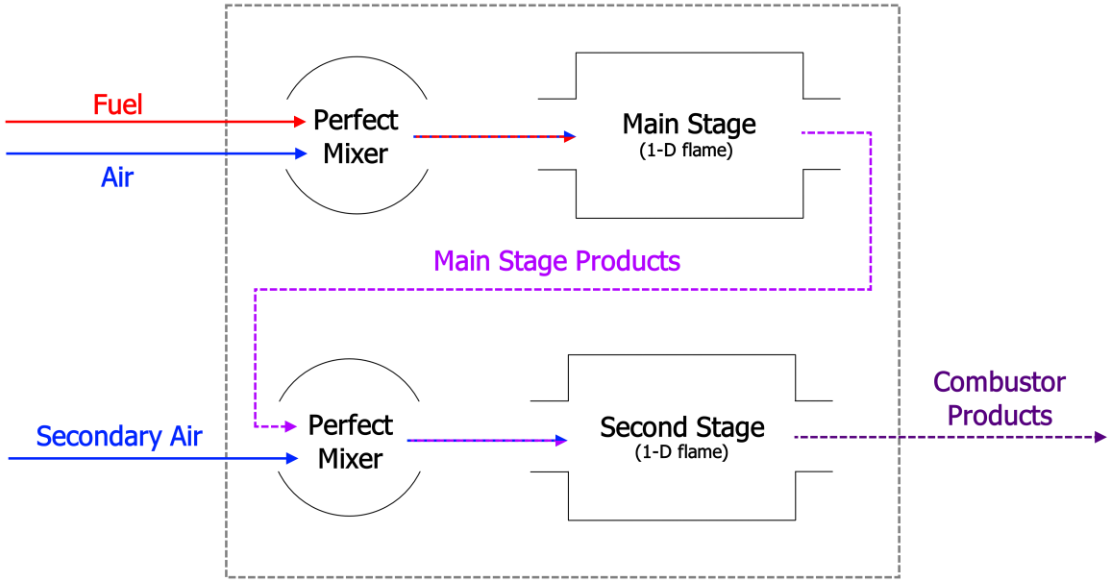




Reactor Network Model

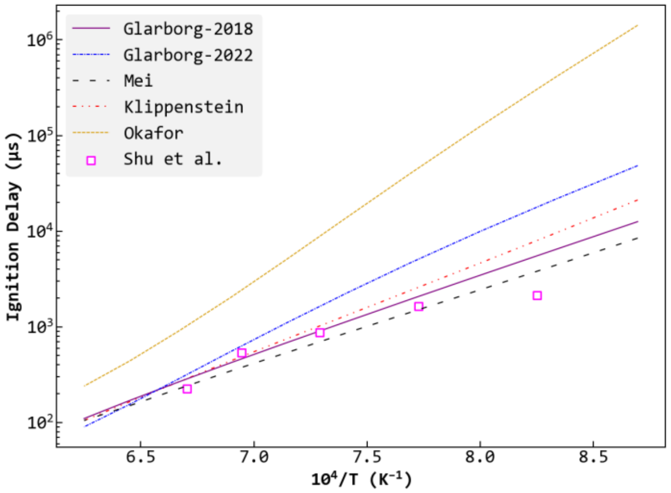
- 1-D flame calculates output for a specified residence time
  - Model calculates in spatial coordinates, conversion to temporal coordinates done after
  - NH_2 peak used to define τ_0 for each stage
- Constants:
  - Fuel: NH_3
  - Oxidizer: 79% N_2, 21% O_2
- Variables:
  - Texit (determined by Φ_{global})
  - Combustor pressure
  - Total residence time, τ_{global}



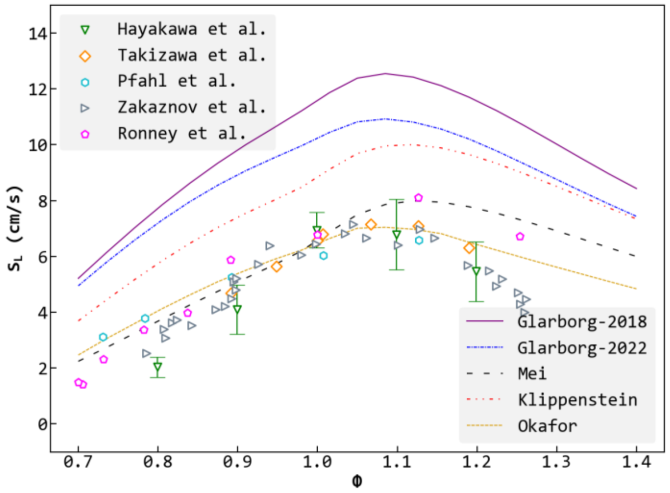
Schematic of staged combustor reactor network model

Reaction Mechanism

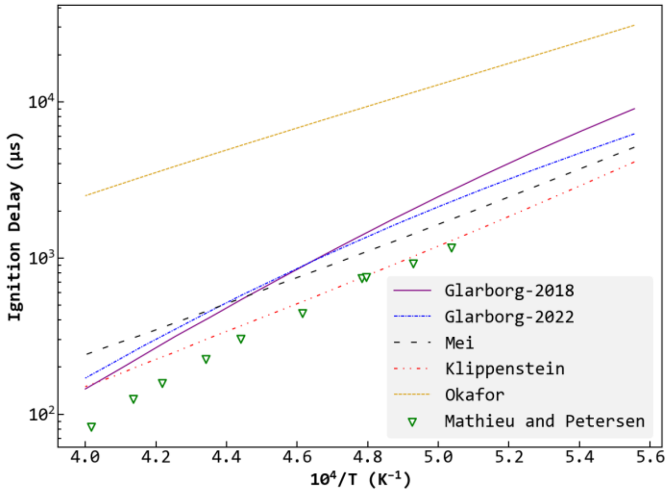
- Compared multiple kinetic models capable of ammonia combustion and NO_x formation
- Chosen mechanism: Mei et al. (2019)
  - Best agreement with experimental datasets
  - Includes all NO_x formation and NH_3 oxidation routes



Sample comparison of ignition delay time (Φ = 0.5, P = 20 bar)



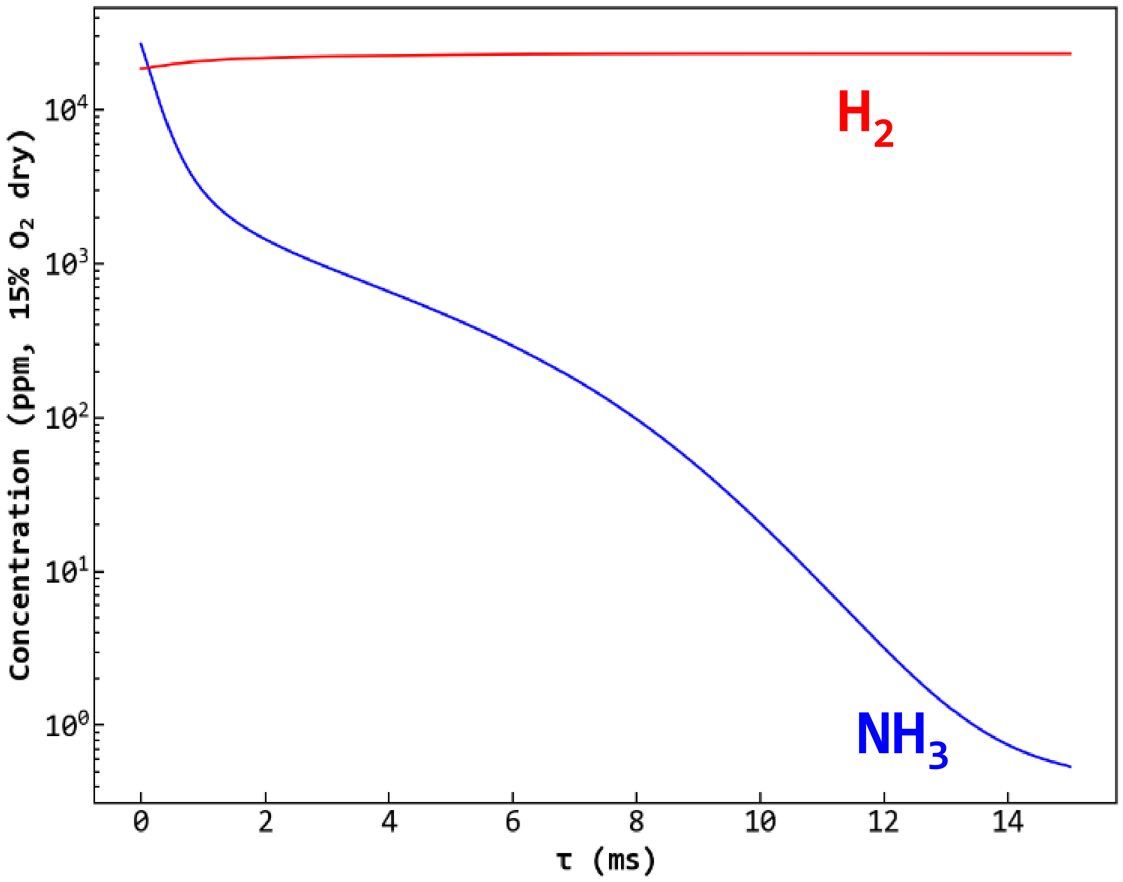
Sample comparison of laminar flame speed (P = 1 bar)



Sample comparison of ignition delay time (Φ = 1.0, P = 1.4 atm; 99% Ar)

Optimization Problem and Constraints

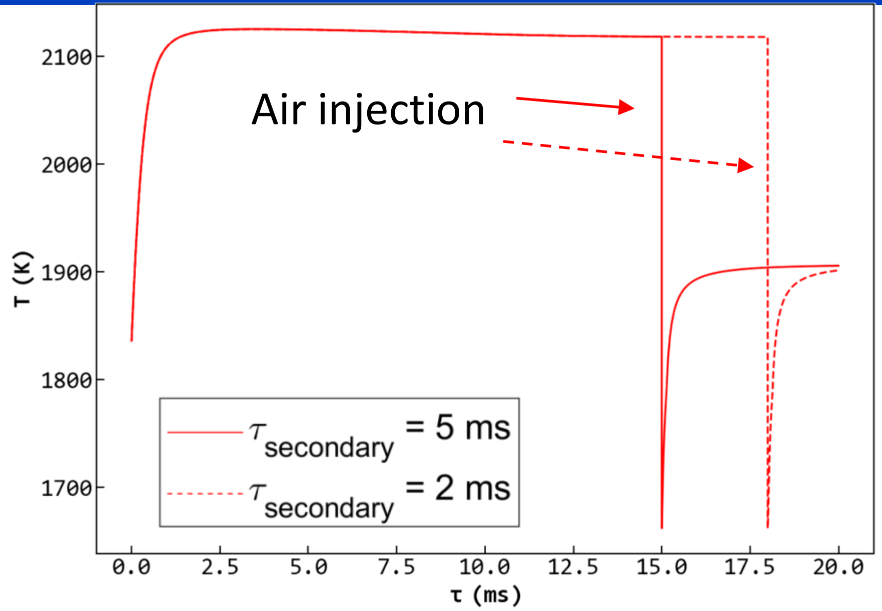
- Parameters: Φ_{main} and τ_{sec}
  - Find optimal parameters that result in minimum NO
- H_2 is a significant product of rich main stage
  - Present at τ_0 since NH_2 peak is used to define start of flame
- Optimizer finds lowest possible τ_{sec} to meet H_2 emissions constraint (combustion efficiency)



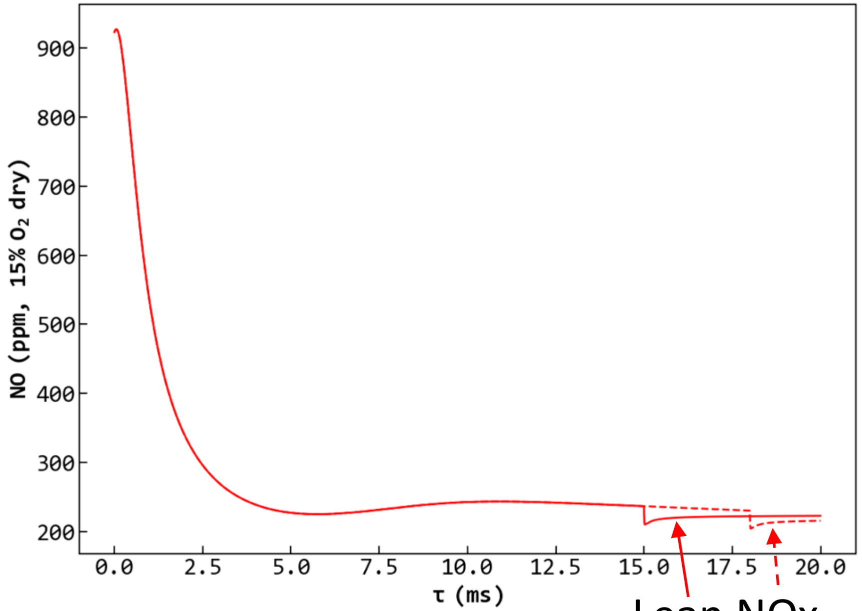
Evolution of NH_3 & H_2 through rich ammonia-air flame (Φ = 1.2, P = 1 bar)

NO Dependence on Φ_{main} and τ_{sec}

- NO emissions sensitive to staging parameters even for fixed Φ_{global} and τ_{global}
- Staging parameters are
  - Φ_{main}
  - $\tau_{secondary}$
- **Example:** NOx vs residence time for two secondary zone residence times
- NOx relaxes towards equilibrium in rich zone
- NOx rises in lean secondary zone
  - Shorter lean zone produces less NOx
  - Lean zone necessary for H_2 burnout (combustion efficiency)



(a) Temperature Profile



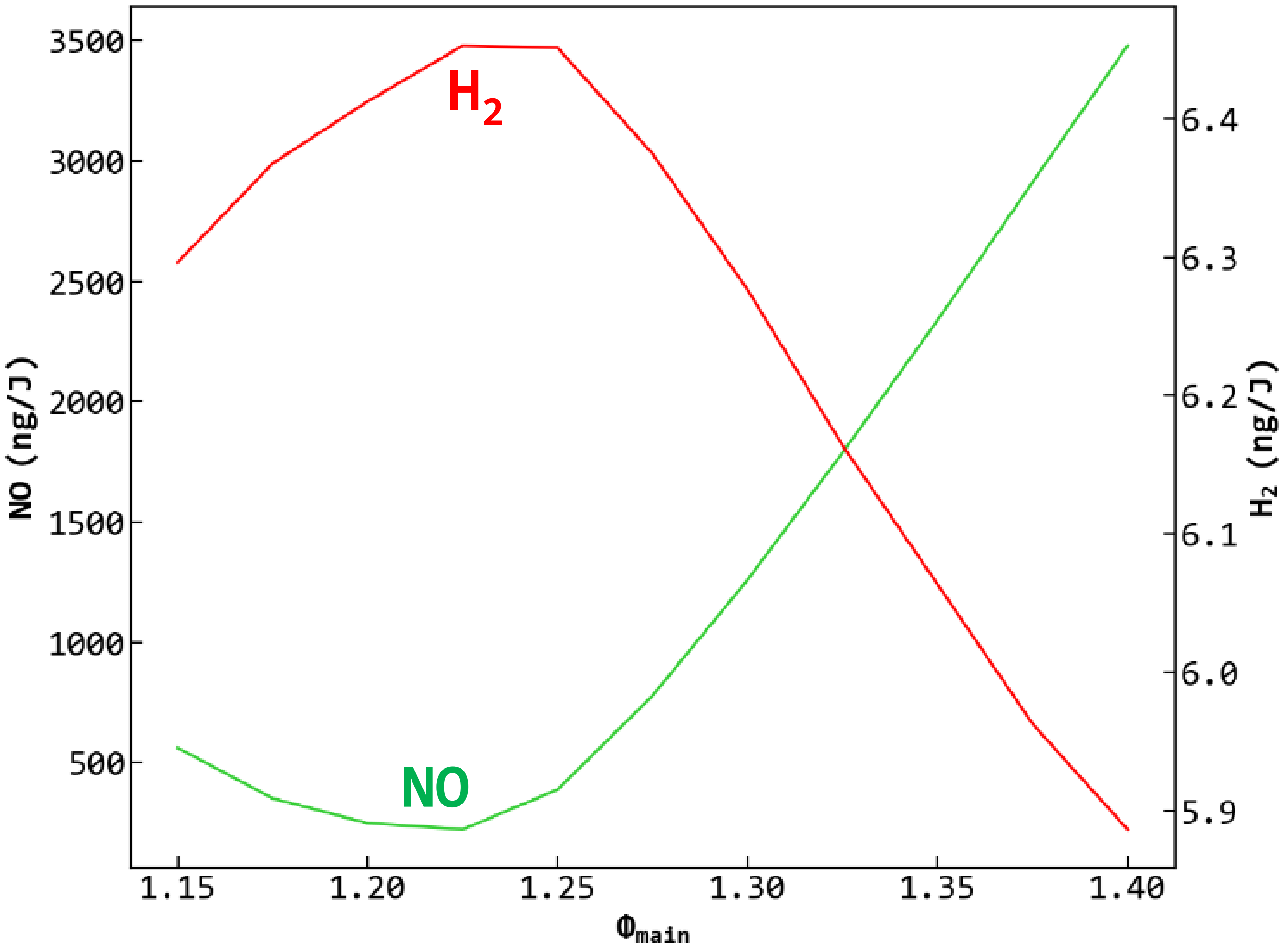
(b) NO Evolution

Lean NOx production

Φ_{main} Dependence

- Example: NO and H2 emissions at fixed Φ_{global}, τ_{global} , and τ_{sec}
- There is an optimum, rich main stage equivalence ratio
- H_2 emission is nearly constant, indicating oxidation can be completed in less than 5 ms for this condition

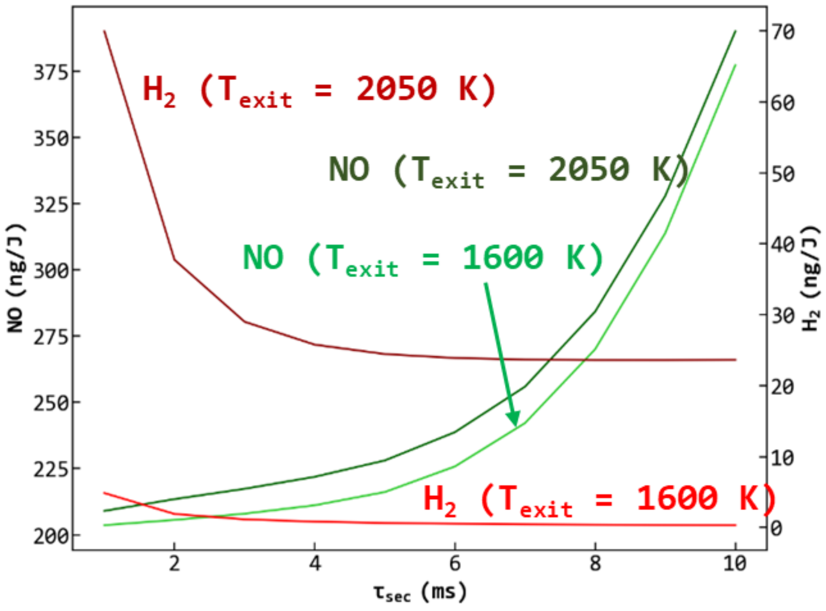
τ_{sec} = 5 ms, P = 1 bar, T_{exit} = 1900 K

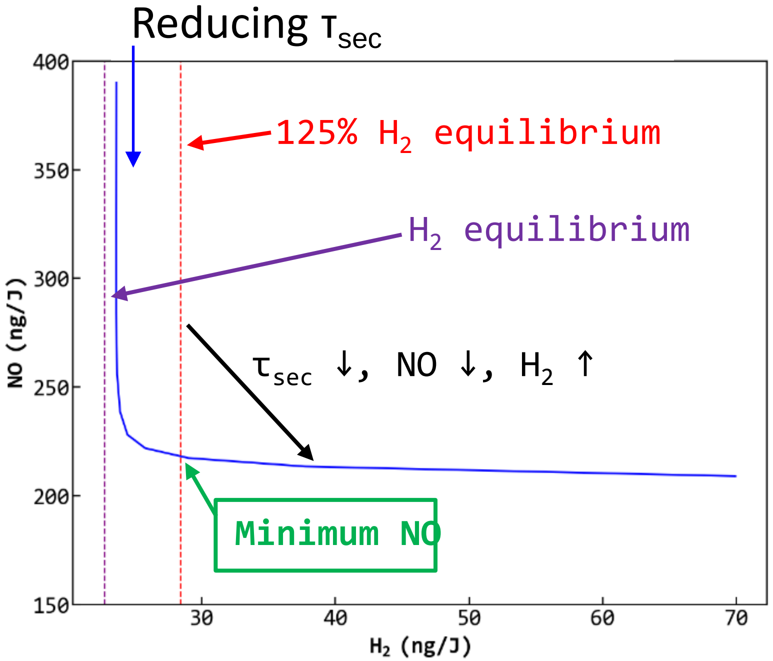


τ_{sec} Dependence

- NO and H_2 have an inverse relationship
  - Long second stage oxidizes H_2
  - Long second stage produces NO

- Objective: shorten τ_{sec} as much as possible within H_2 constraint
  - Example for T_{exit} = 2050 K
  - In this example, τ_{sec} = 3 ms is optimal

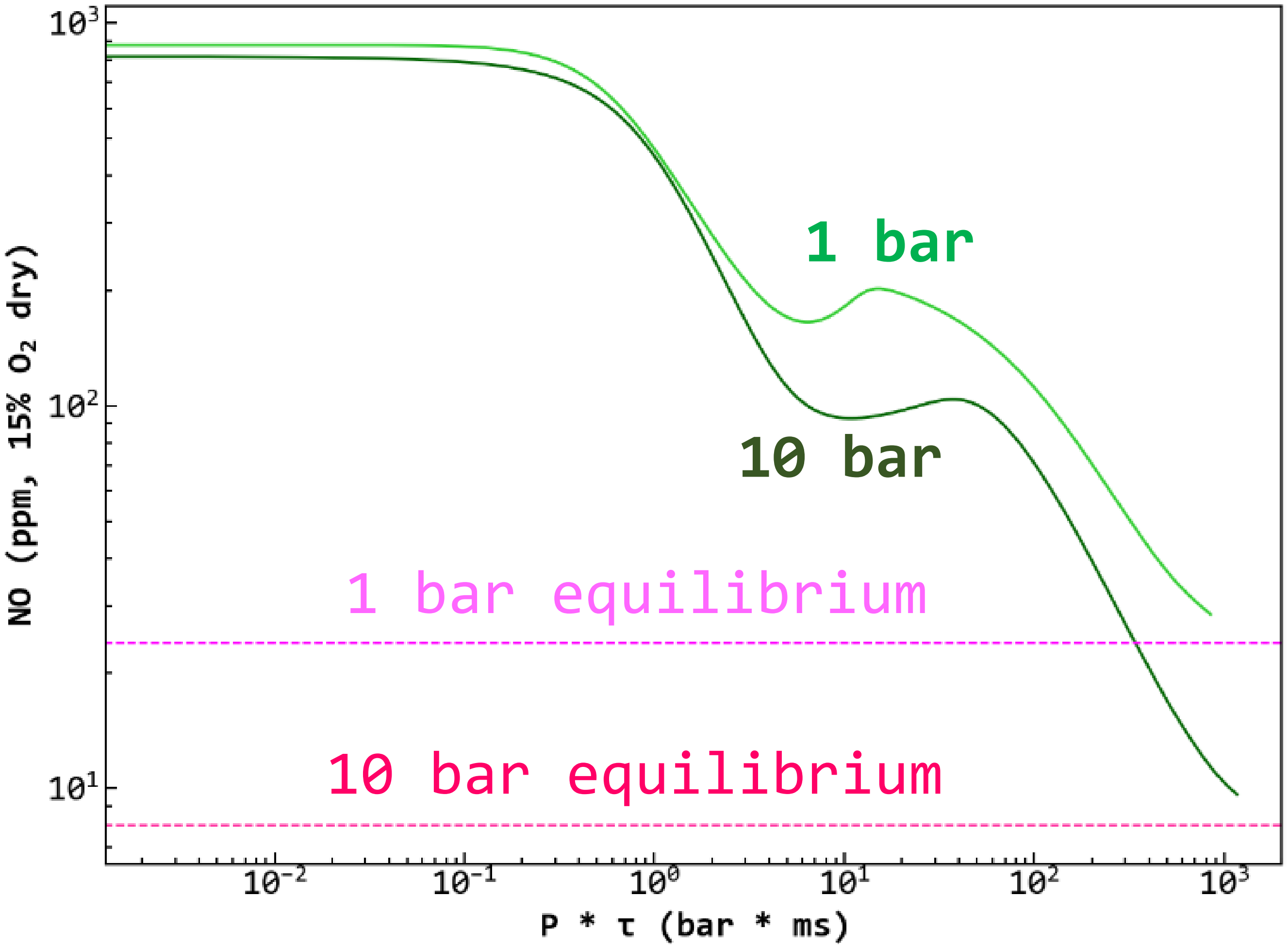




$^*\Phi_{main}$ = 1.22, P = 1 bar

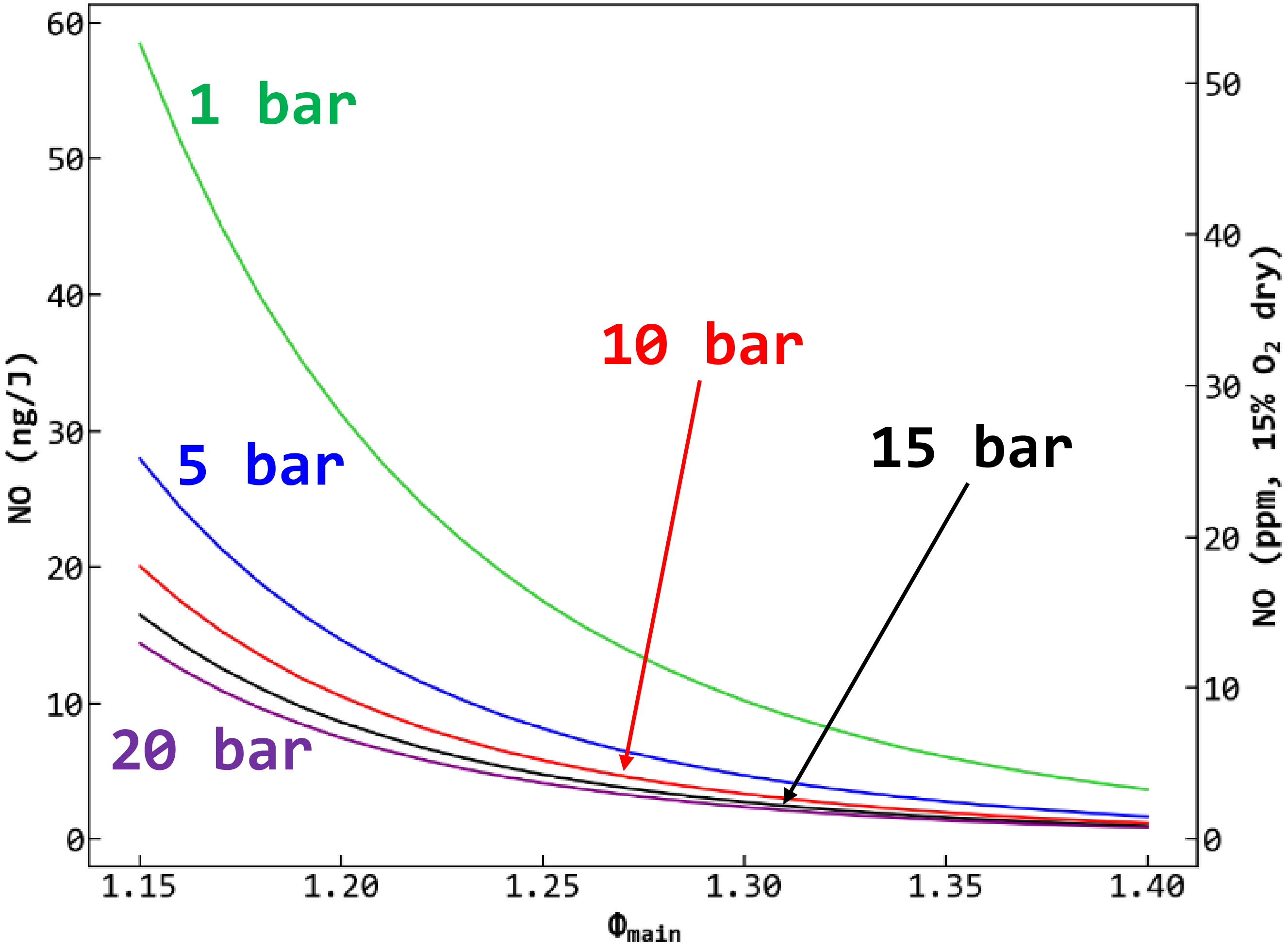
NO Production Sources

- Unrelaxed main stage NO can be a significant NO_x contribution
- Residence time required for equilibrium much larger than current practical combustor designs
  - 1000 ms at 1 bar
  - 100 ms at 10 bar
  - Pressure helps
- Two step relaxation due to OH formed in rich main stage reacting with N and NH to form NO



NO Production Sources

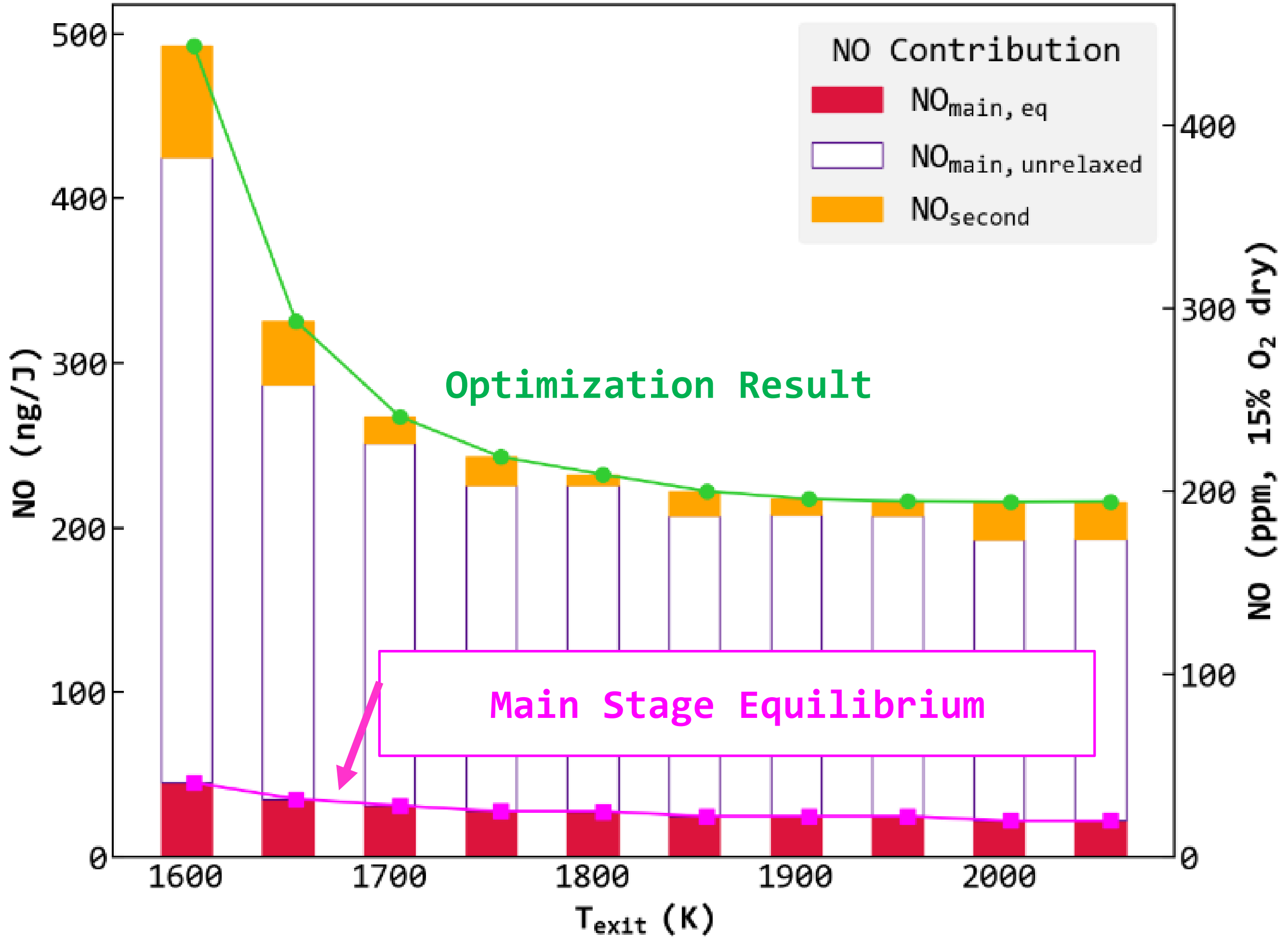
- High pressure and richer main stage will drive $NO_{eq,main}$ down
- Observation: achieving equilibrium NOx in rich main stage enables very low NOx
  - Lean secondary zone NOx must be limited
  - *What is the main source of NO emissions in ammonia RQL*?



Combustor Firing Temperature Sensitivities

- Majority of NO contribution is from $NO_{main,unrelaxed}$
- Firing temperature helps: faster main stage NO relaxation
- Longer main stage would help

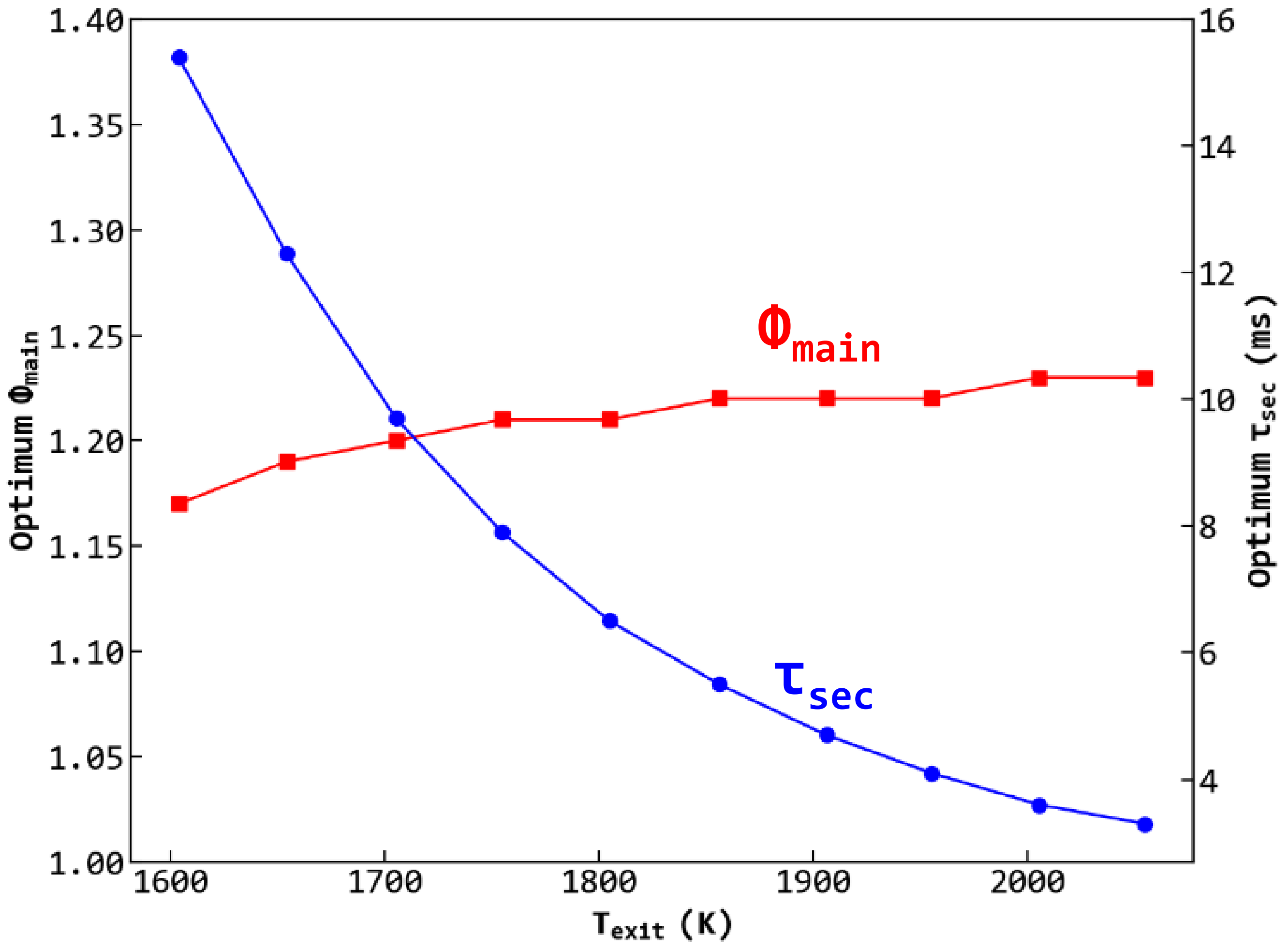
Total NOx = Main Stage + Unrelaxed + Secondary



*P = 1 bar; τ_{global} = 20 ms

Combustor Firing Temperature Sensitivities

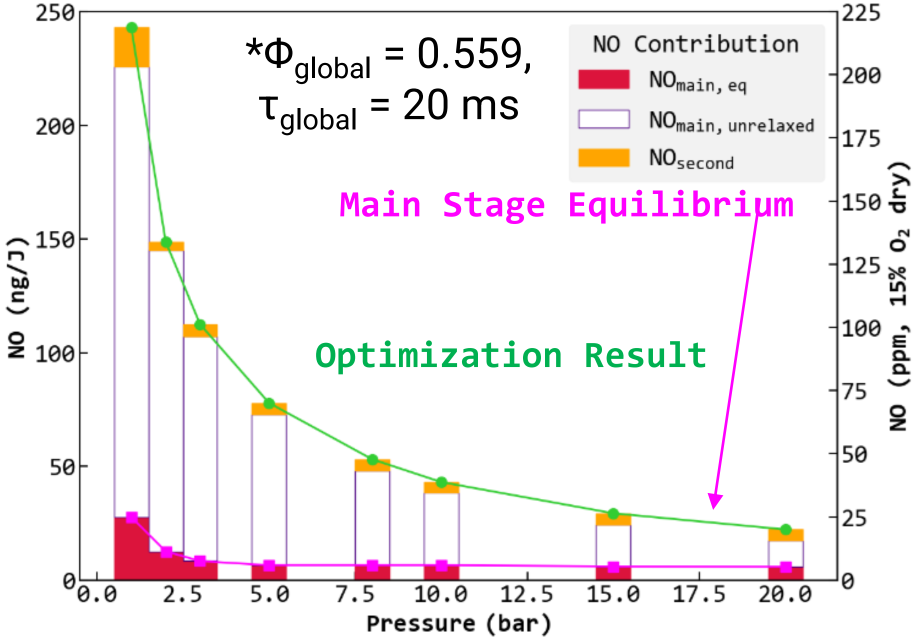
- Richer main stage beneficial (lower equilibrium NO)
- Relaxation toward equilibrium faster with hotter main stage
- Higher temperatures allow for faster H_2 oxidation
  - Shorter τ_{sec}
  - Helps with Zeldovich NOx



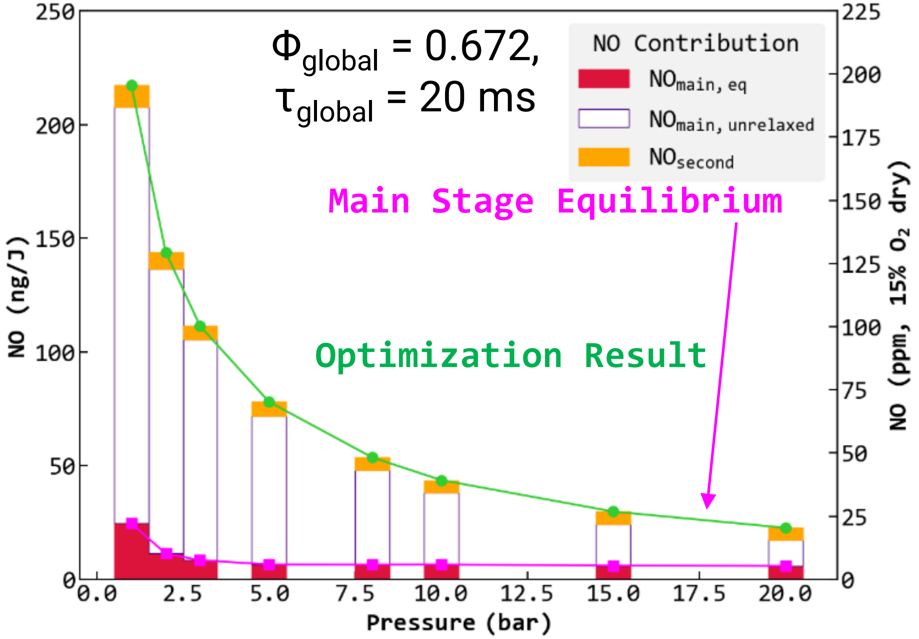
Optimized parameters for minimum NO at various firing temperatur

Combustor Pressure Sensitivities

- High pressure allows main stage to approach equilibrium faster
- Firing temperature more sensitive at lower pressures



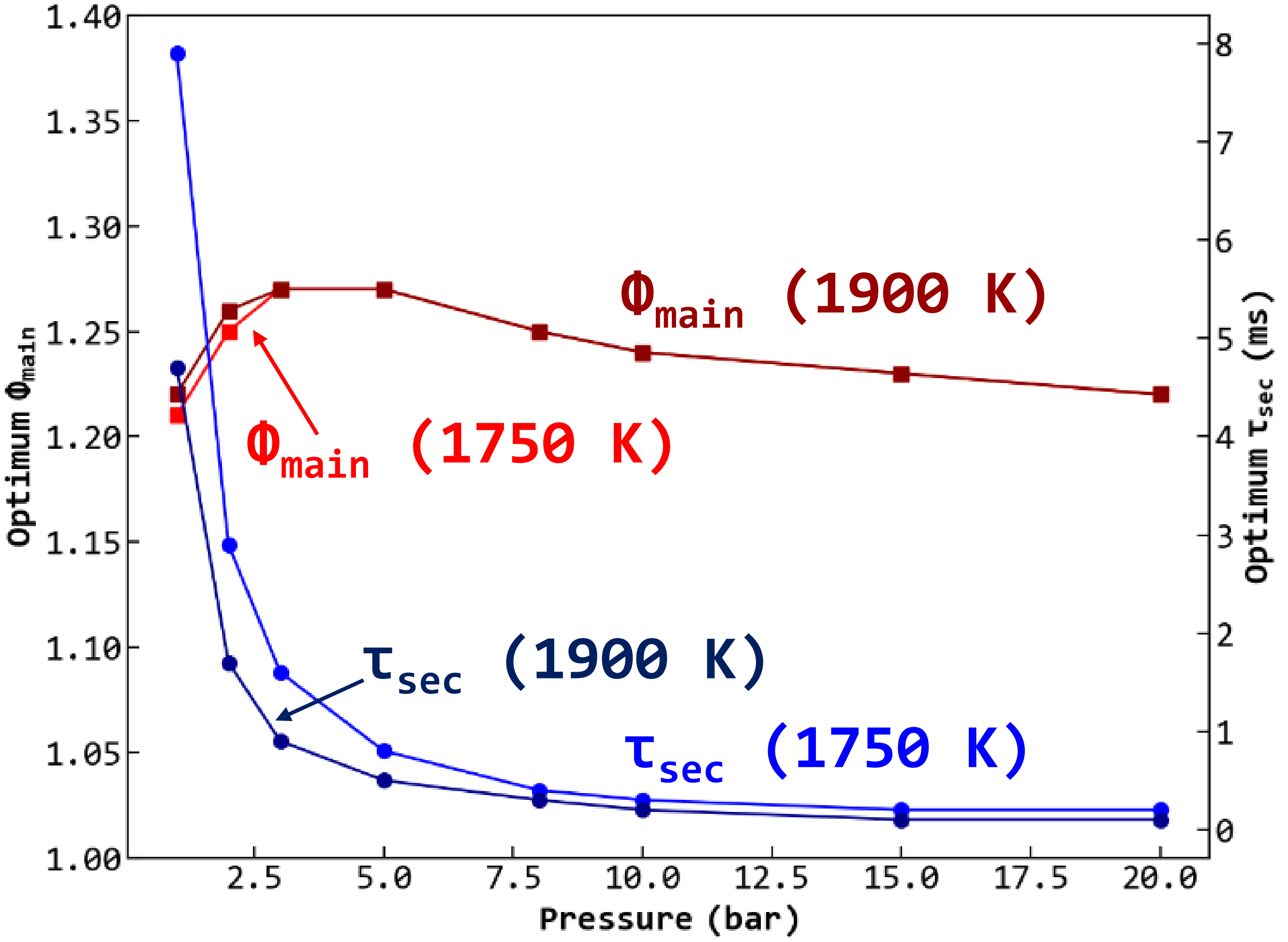
(a) T_{exit} = 1750 K



(b) T_{exit} = 1900 K

Combustor Pressure Sensitivities

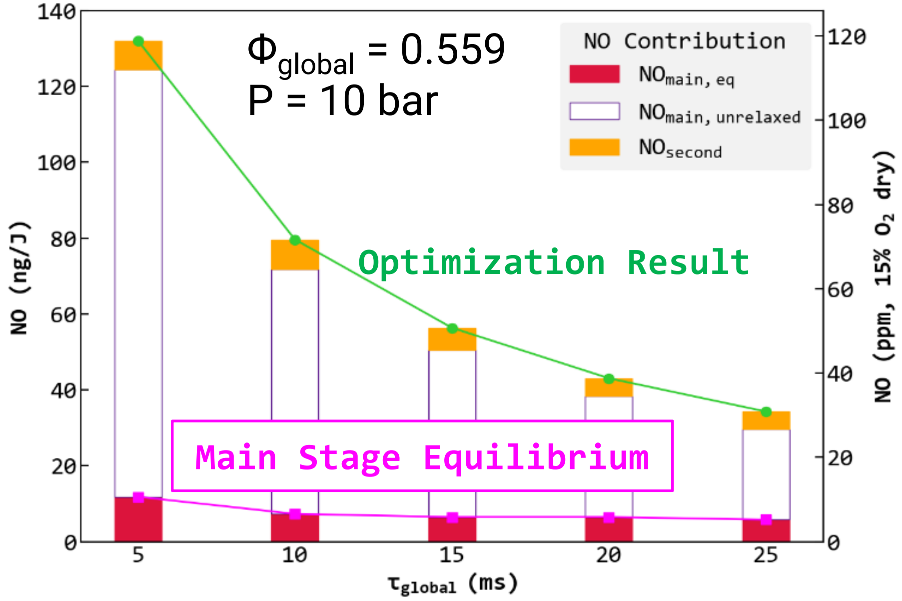
- Optimal Φ_{main} and τ_{sec} are independent of firing temperature at high pressure



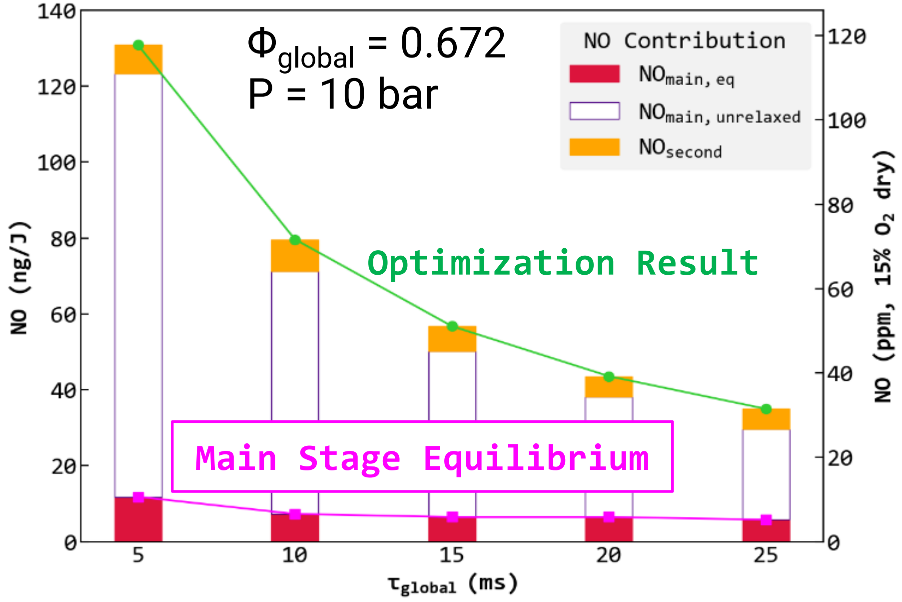
Optimal parameters for minimum NO at varying combustor pressure

Global Residence Time Sensitivities

- Longer combustor residence time helps
- Main stage NO can relax towards equilibrium



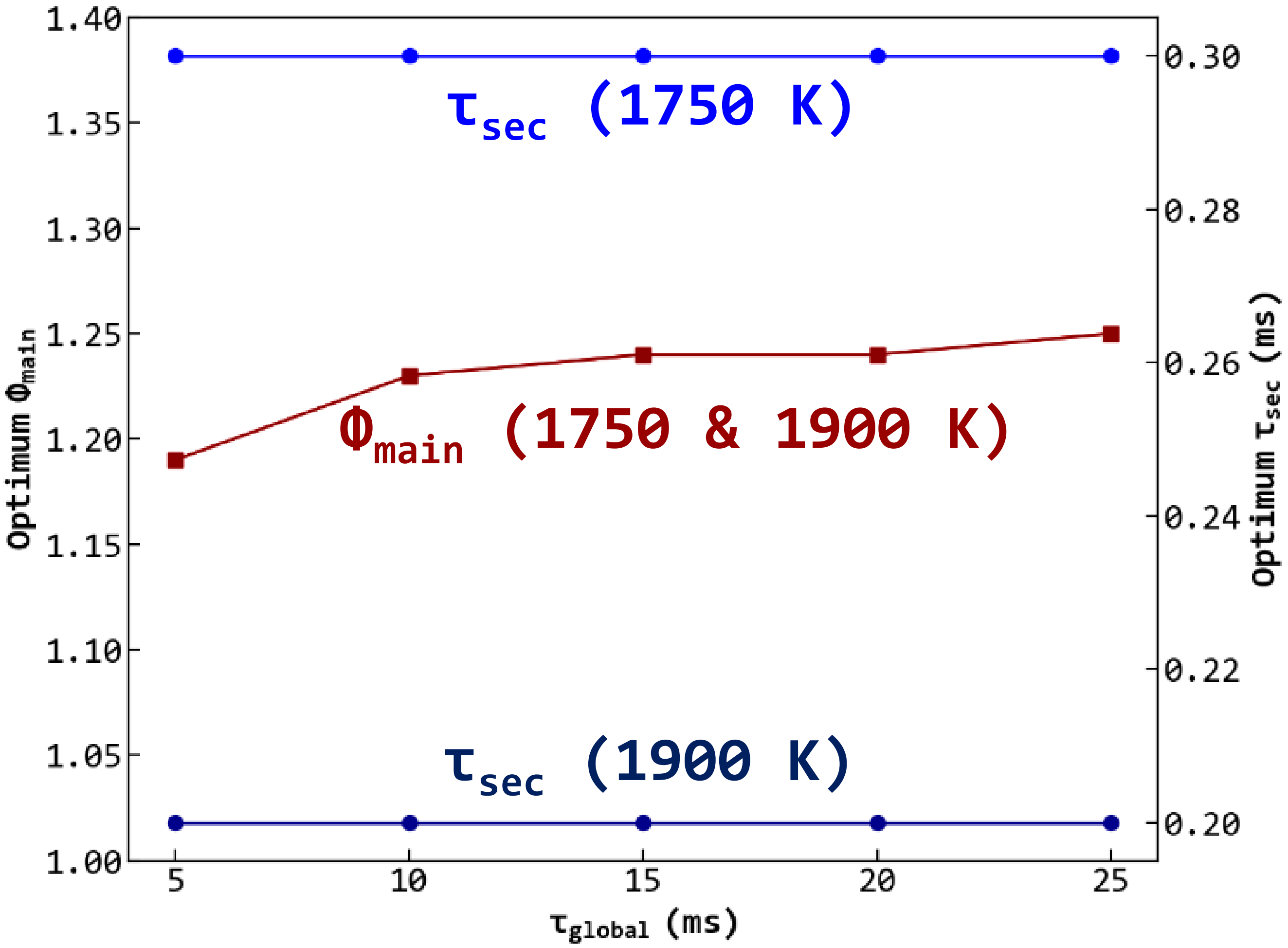
(a) T_{exit} = 1750 K



(b) T_{exit} = 1900 K

Global Residence Time Sensitivities

- Optimum Φ_{main} same for all conditions (high pressure)
- Optimal τ_{sec} independent of global residence time
  - All added residence time is main stage, reducing $NO_{main,unrelaxed}$



Conclusions

- Theoretical minimum NOx emissions below 30 ppm are possible for ammonia combustion with RQL
- Intuition for NOx formation from lean premixed combustion is not applicable here
- Low NOx rich main stage (relax to equilibrium):
  - High temperature
  - High pressure
  - Long residence time
- Low NOx secondary stage:
  - Low residence time
  - Sufficient residence time to burn out H_2 for combustion efficiency
- Significant engineering required to navigate real world effects and approach these limits

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