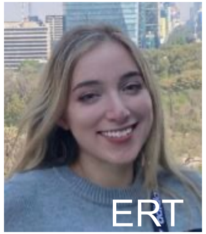
Ammonia combustion in inert porous media burners: systematic experimental characterization and chemical kinetics analysis

G.Vignat, T. Zirwes, E. R. Toro, E. Boigné, D. Trimis, M. Ihme



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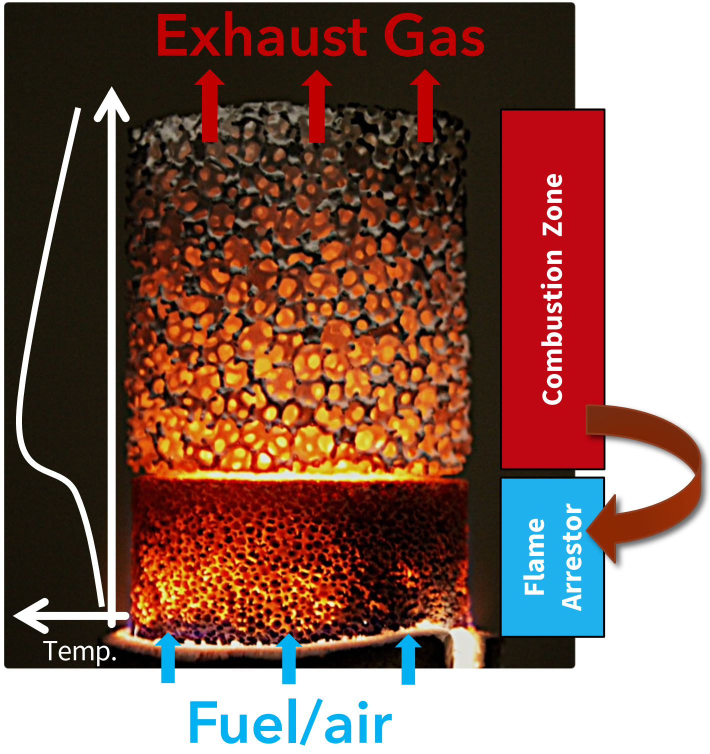
Porous media combustion



Applications in:

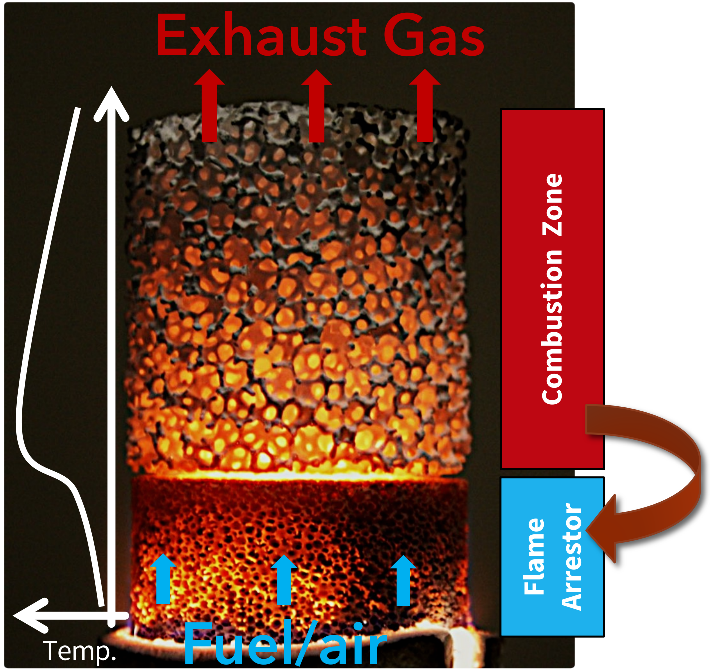
- Gas turbines
- Domestic boilers
- Radiant industrial heaters

Heat recirculation through solid matrix:

- Pre-heats fresh reactants
- Increases the flame speed

Ellzey et al., *Prog. Energy Combust. Sci.* 72 (2019).
Wood and Harris, *Prog. Energy Combust Sci.* 34 (2008).
Trimis and Durst, *Combust. Sci. Technol.* 121 (1996).
Sobhani et al., *Proc. Combust. Inst.* 37(4) (2019).

Porous media combustion



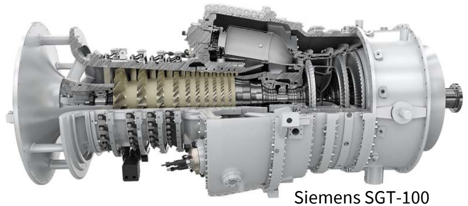
Key concept: Internal Heat recirculation by heat-conducting solid-ceramic matrix

- Extended power modulation
- Low noise emission
- Reduction in CO, NO, unburnt fuel
- Fuel-flexible operation
- Combustion of ultra-lean fuel/air mixtures
- No thermo-acoustic instabilities

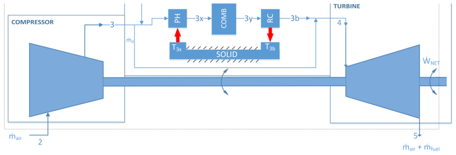
Benefits of porous media combustion

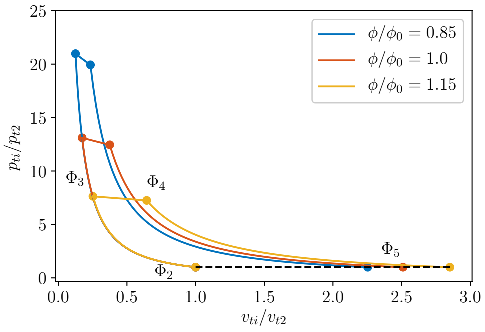
Thermodynamic cycle analysis

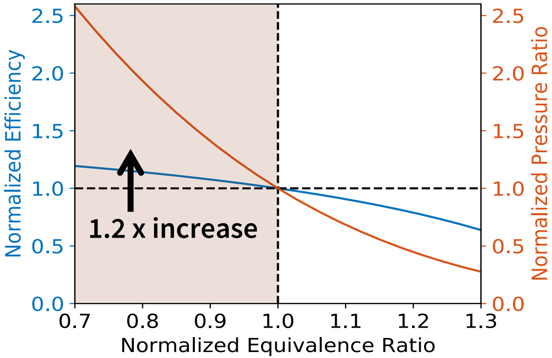
- Replace primary combustion zone with PMC
- Extended lean flammability limit
  - ➔ Increase compression ratio
  - ➔ increase thermal efficiency by 20%
  - ➔ reduce emissions of NO_x by 50%

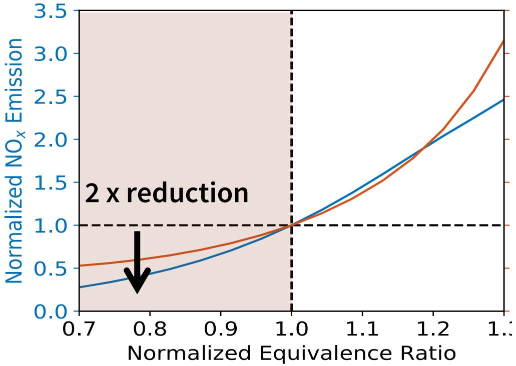


Siemens SGT-100







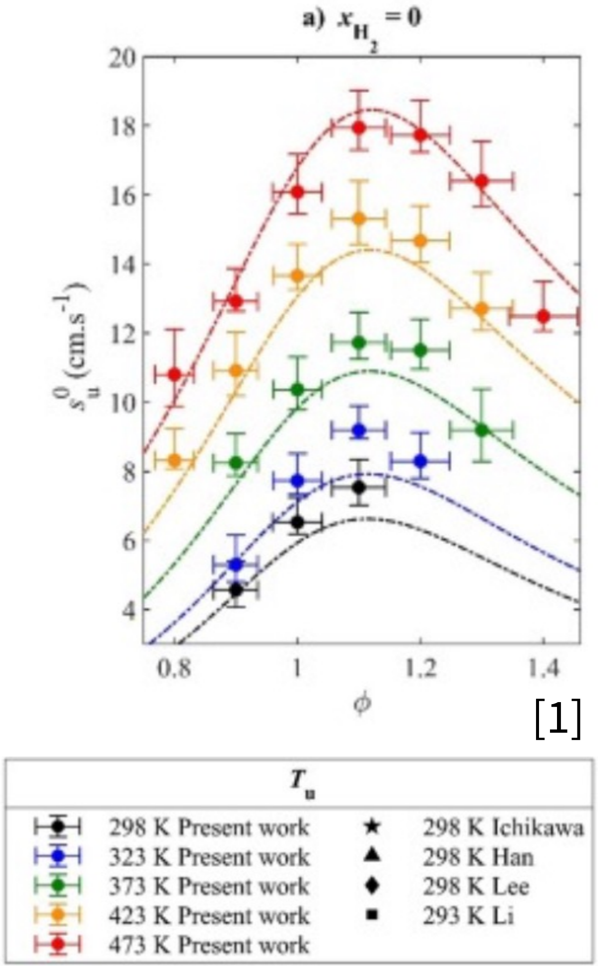


Mohaddes, Ihme and Chang , "Superadiabatic Matrix-Stabilized Combustion for Gas Turbine Engine Performance Improvement," Applied Energy, 2020

Why PMBs for ammonia?

Heat recirculation through solid matrix [2,3]:

- Pre-heats fresh reactants
- **Increases the flame speed**
- **Enables very lean/rich combustion**
  - › **Reduced pollutant emissions**
  - › **Improved thermodynamic efficiency [4]**



[1]

[1] Lhuillier et al., *Fuel* 263 (2021).
[2] Ellzey et al., *Prog. Energy Combust. Sci.* 72 (2019).
[3] Masset et al., *Combust. Theory Model.* 25 (2021).
[4] Mohaddes et al., *Energy* 207 (2020).

Why PMBs for ammonia?

Computational design optimization

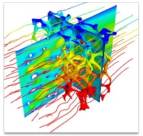
Mass conservation: $\frac{\partial(\rho_g\epsilon)}{\partial t}+\frac{\partial(\rho_g u\epsilon)}{\partial x}=0$

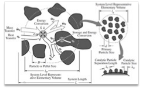
Species conservation: $\rho_g\epsilon\frac{\partial Y_i}{\partial t}+\rho_g\epsilon u\frac{\partial Y_i}{\partial x}+\frac{\partial}{\partial x}(\rho_g\epsilon Y_i V_i)-\dot{\omega}W_i\epsilon=0$

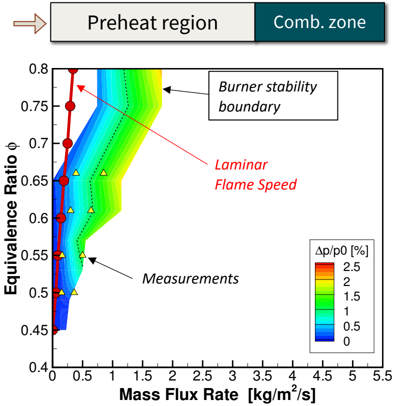
Energy conservation:

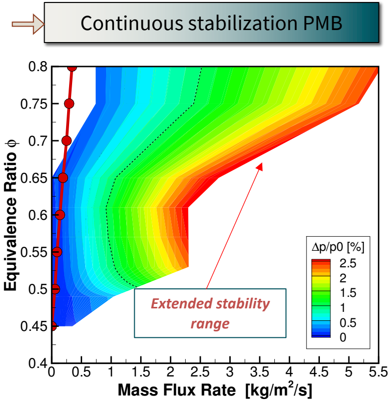
$$\rho_g\epsilon C_g\frac{\partial T_g}{\partial t}+\rho_g\epsilon C_g u\frac{\partial T_g}{\partial x}+\epsilon\sum_{i=1}^{n}\rho_{g,i}C_{g,i}V_iY_i\frac{\partial T_g}{\partial x}+\epsilon\sum_{i=1}^{n}\dot{\omega}_i h_i W_i-\frac{\partial}{\partial x}\left(k_{g,eff}\epsilon\frac{\partial T_g}{\partial x}\right)+h_v(T_g-T_s)=0$$

Solid temperature: $\rho_s C_s\frac{\partial T_s}{\partial t}+\frac{\partial}{\partial x}\left(\lambda_s\frac{\partial T_s}{\partial x}\right)+\frac{dq}{dx}-h_v(T_g-T_s)=0$



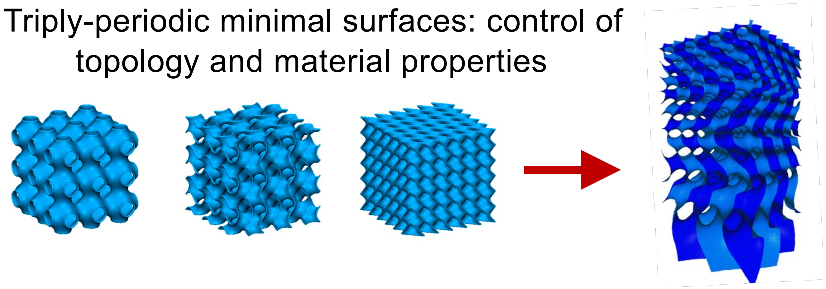




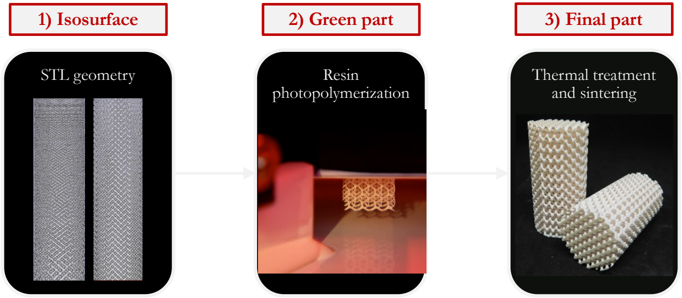


Tailoring porous-ceramic foams

Triply-periodic minimal surfaces: control of topology and material properties

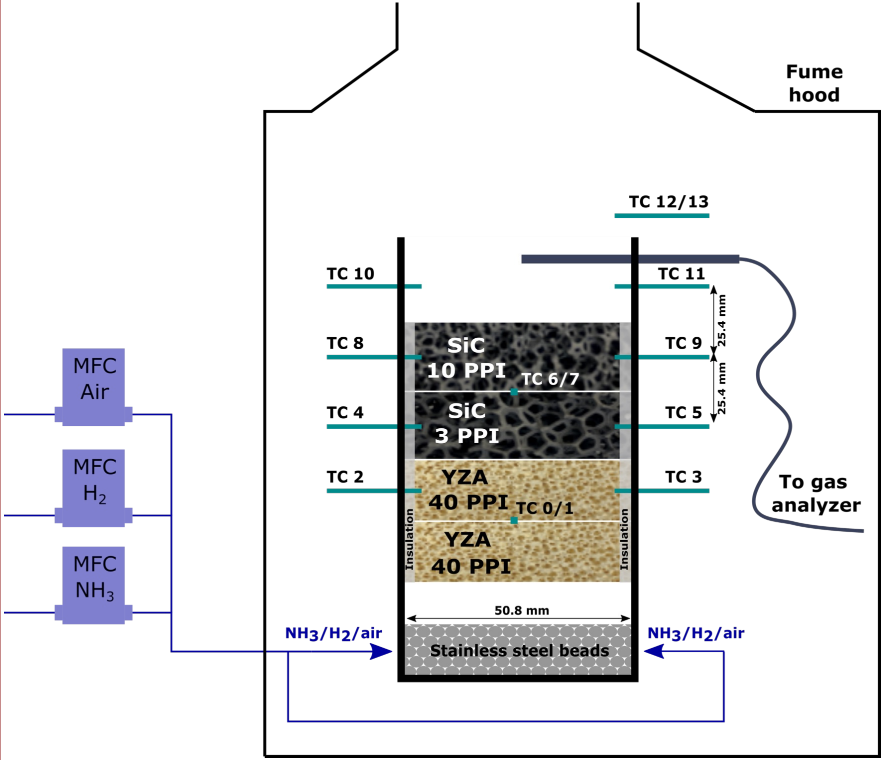


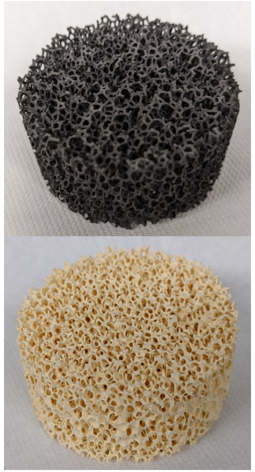
Additive Manufacturing Ceramics



Sobhani *et al.* Tailoring Ceramic Porous Structures Applied to High-Temperature Applications, Adv. Eng. Mat. 2020

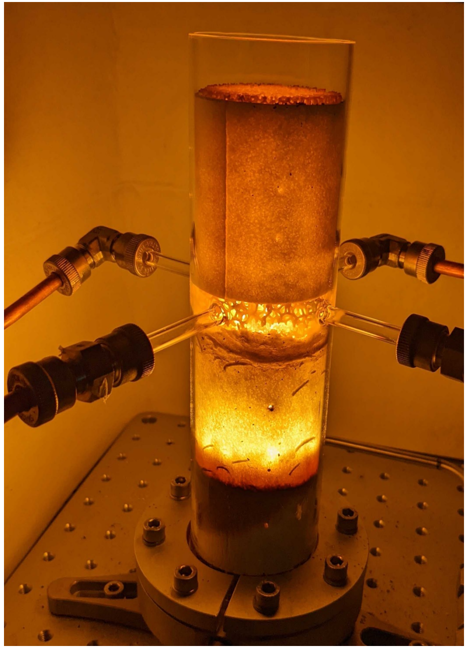
Experimental setup: Interface stabilized PMB





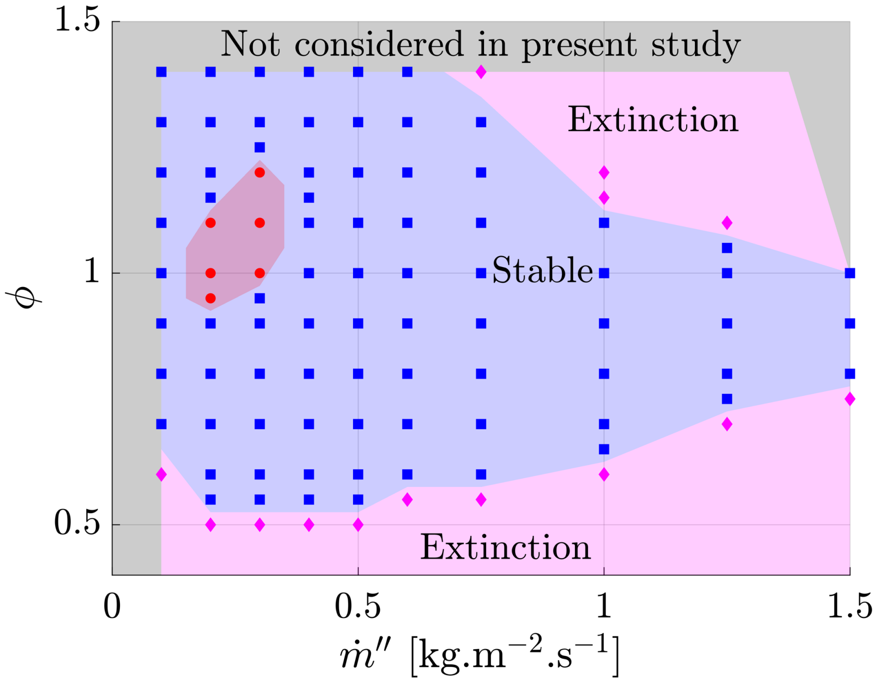
Combustion
Heat recirculation

Flame Arrestor



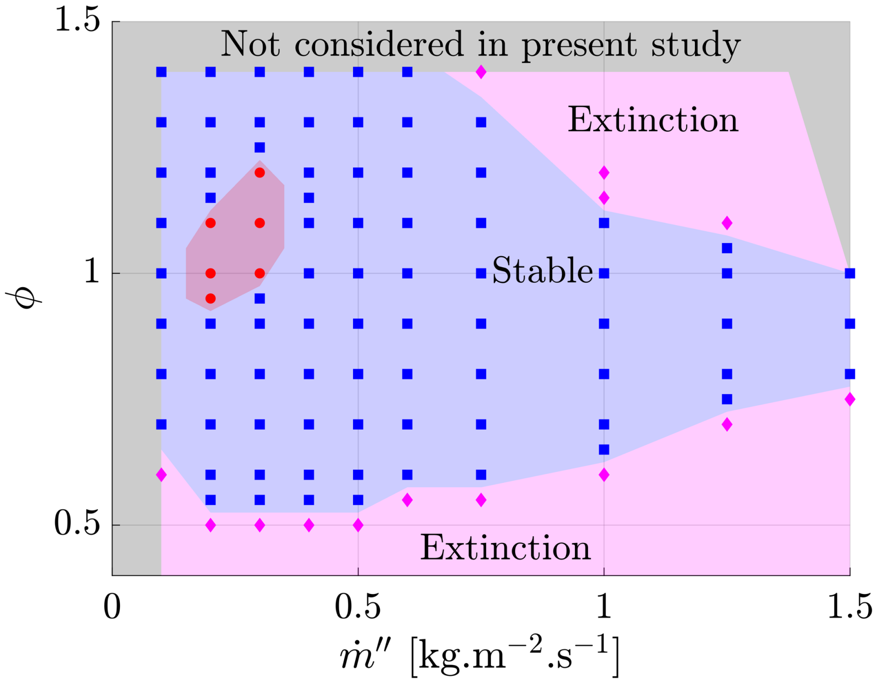
Trimis, Durst, *Combust. Sci. Technol.* 121 (1996).

Extended flame stabilization

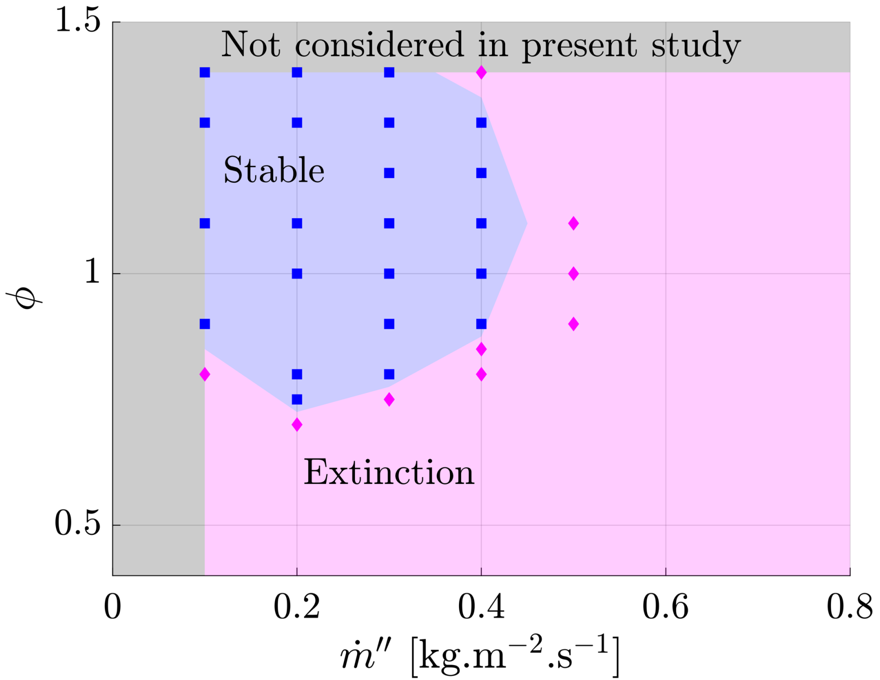


- Results for a $x_{NH_3} = 0.7$, $x_{H_2} = 0.3$ mixture
- Extended stability region, from:
  - Lean: $\phi_{LBO} = 0.55$
  - To rich conditions: $\phi = 1.4$
- Turndown ratio greater than 15:1
- Power density up to 62 MW.m^{-3}
  - Estimated 5 to 24 MW.m^{-3} for swirl flames at atmospheric pressure

Extended flame stabilization: pure NH_3 operation



$x_{NH_3} = 0.7, x_{H_2} = 0.3$



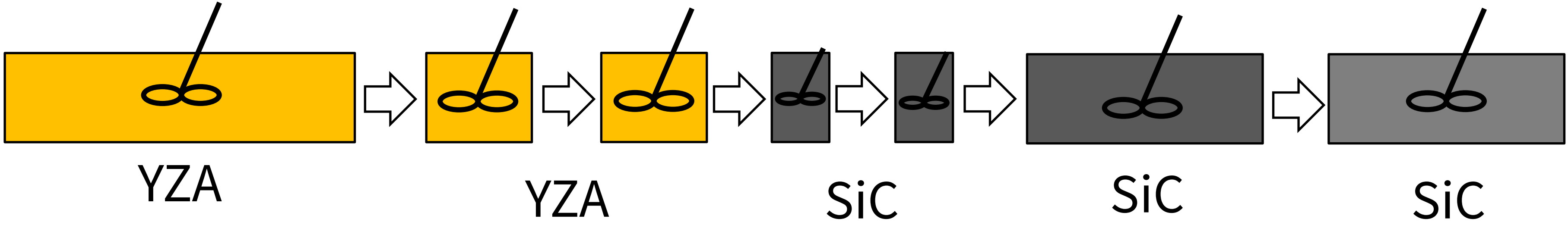
$x_{NH_3} = 1$

0D reactor network for PMB

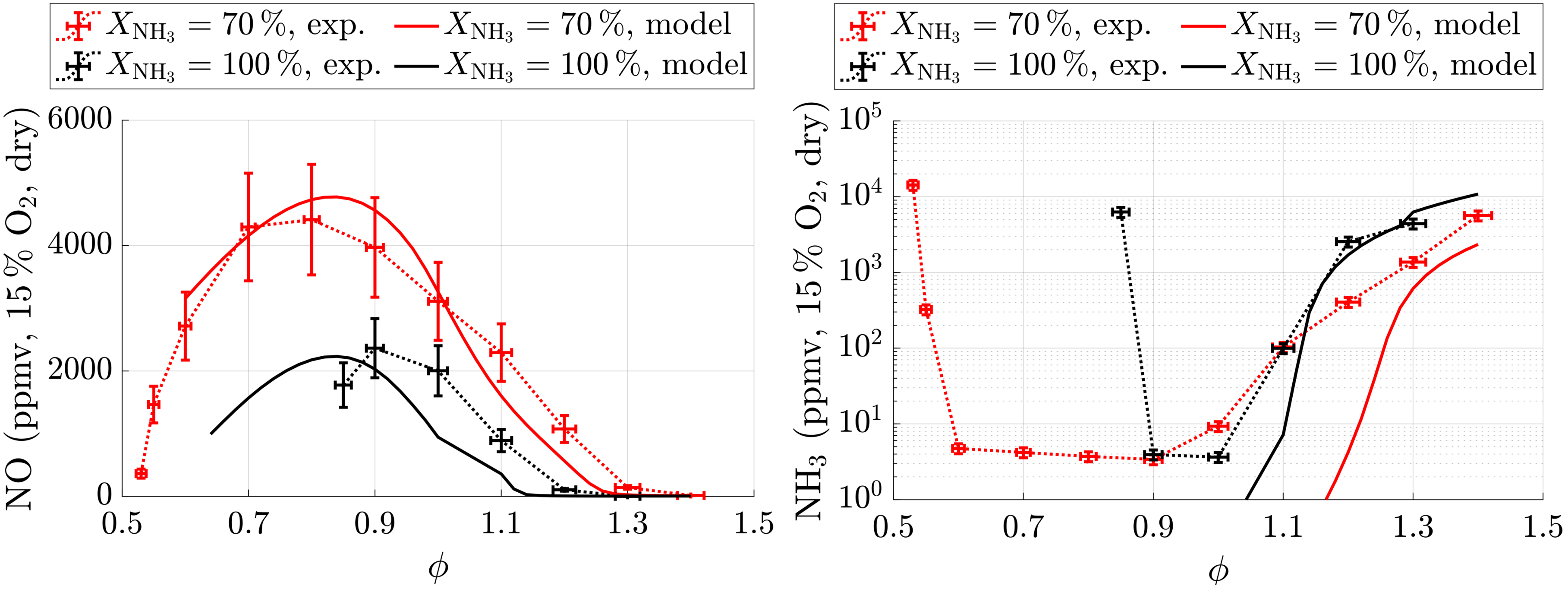
Cantera

7 continuously stirred **reactor network model extended with interphase** (solid-gas) heat transfer

- Reaction mechanism by Stagni et al., *Reac Chem Eng* 5(4), 2020.
- Interphase heat transfer (Bedoya et al., *Combust Flame* 162, 2015)
- **Effective material properties computed from x-ray tomographies**
- Inter-reactor heat transfer including radiation and conduction

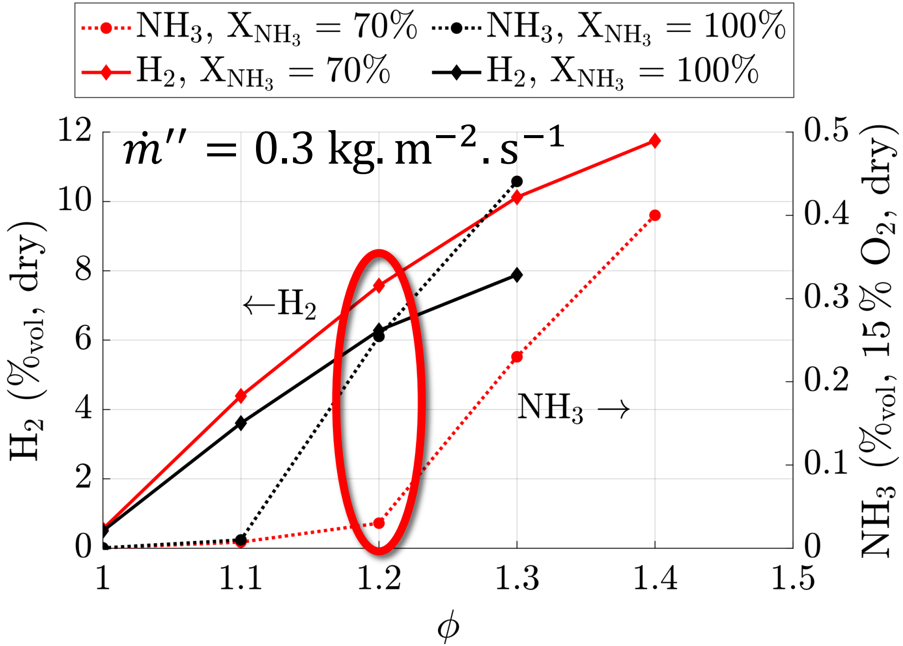


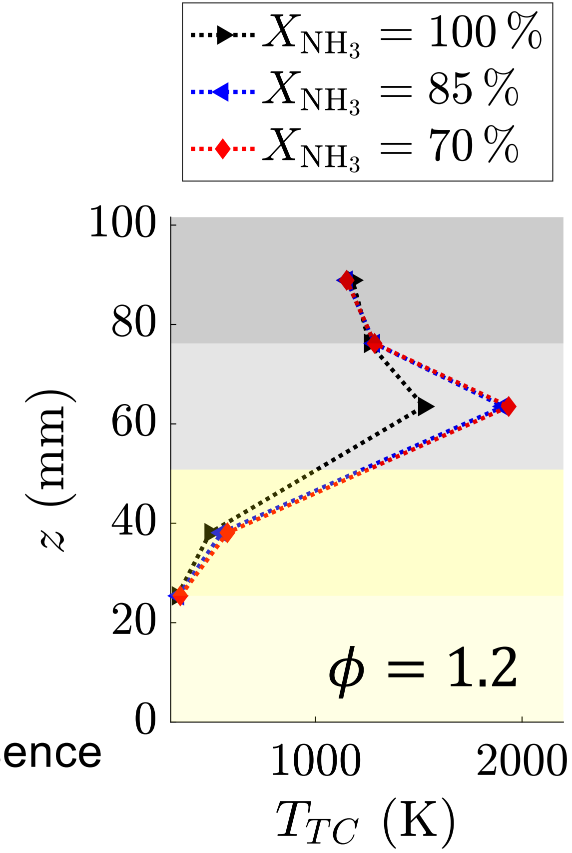
Burner pollutant emissions and model validation



- Results for $\dot{m}'' = 0.3\ \mathrm{kg.m^{-2}.}s^{-1}$
- The reactor network model captures NO emissions to good accuracy.
- Model breaks for weakly stabilized flames in the very lean region.

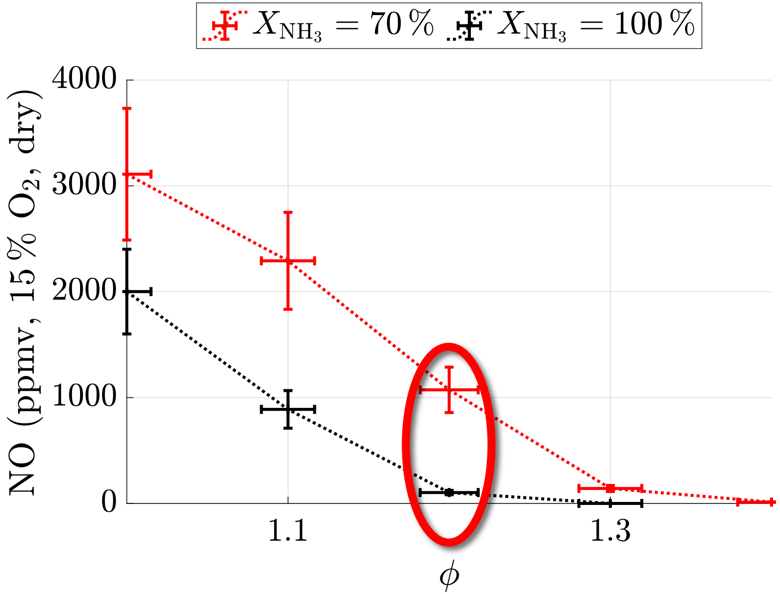
Exhaust composition in the rich regime: H_2/NH_3 ratio

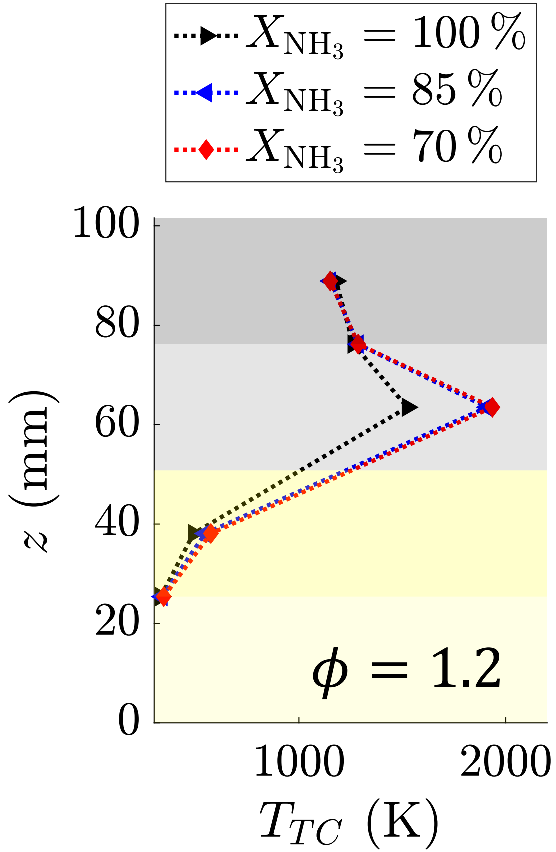




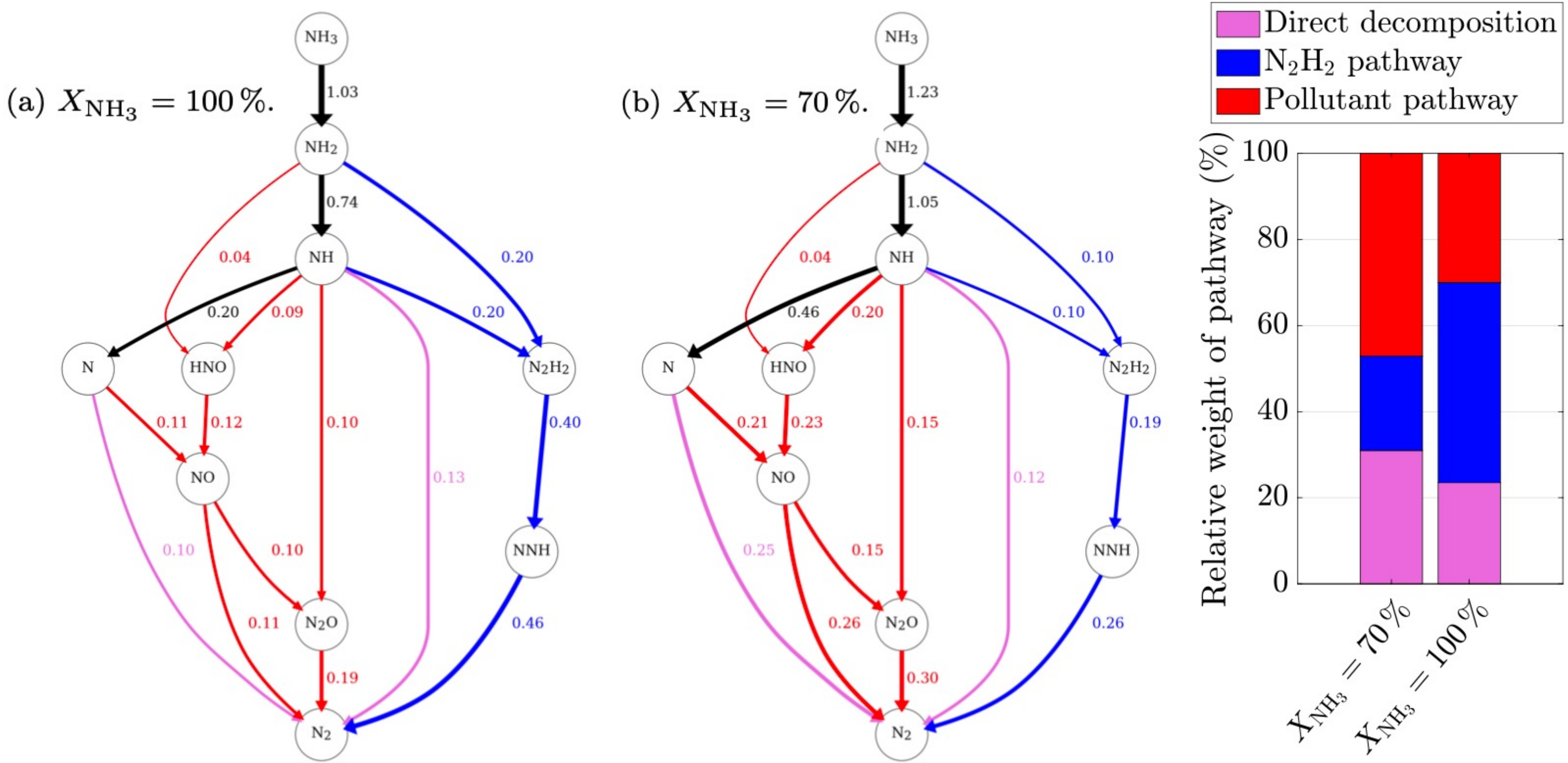
- High conversion of NH_3 to H_2 in rich conditions
- $\phi = 1.2$: a ~100 K difference in burner temperature explains the lower consumption rate of NH_3 and presence of unburnt in the exhaust stream (reactor network)

Exhaust composition in the rich regime: NO emissions



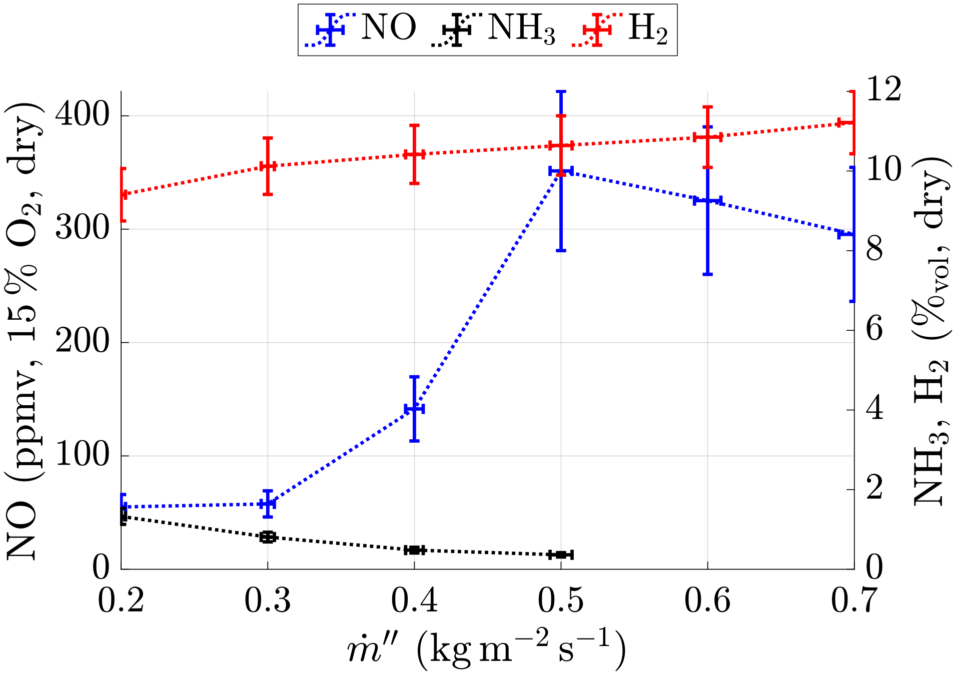


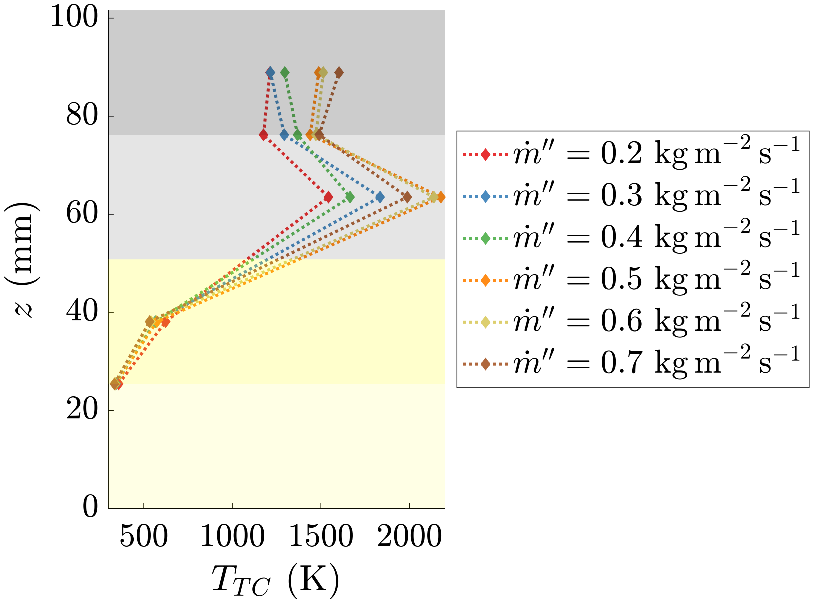
- Constant mass flux: $\dot{m}'' = 0.3\ \mathrm{kg.m^{-2}.s^{-1}}$
- Fast decrease of NO emissions with increasing ϕ
- Emissions systematically lower for pure NH_3



- 2 factors combine to explain lower NO emissions for the X_{NH_3}:
  - Lower NO formation rates in the flame region
  - Unburnt NH3 and NH2 in the post-flame region

Emissions at rich conditions: effect of mass flux





- Mass flux has a small influence on pollutant emission
- Increasing reforming efficiency with increasing mass flux
- Increasing NO emissions correlated with increasing operating temperatures

1D simulation framework

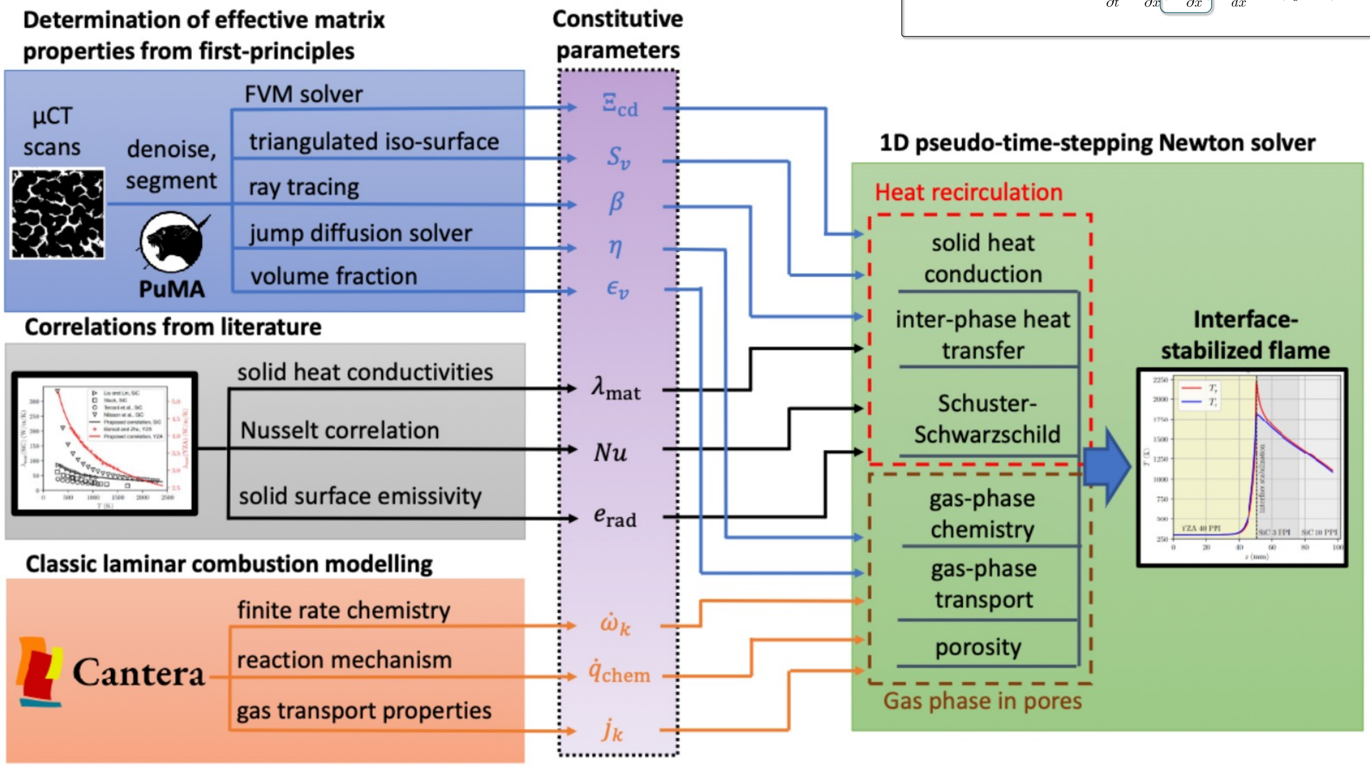
Mass conservation: $\frac{\partial(\rho_g \epsilon)}{\partial t} + \frac{\partial(\rho_g u \epsilon)}{\partial x} = 0$

Species conservation: $\rho_g \epsilon \frac{\partial Y_i}{\partial t} + \rho_g \epsilon u \frac{\partial Y_i}{\partial x} + \frac{\partial}{\partial x}(\rho_g \epsilon Y_i V_i) - \dot{\omega} W_i \epsilon = 0$

Energy conservation:

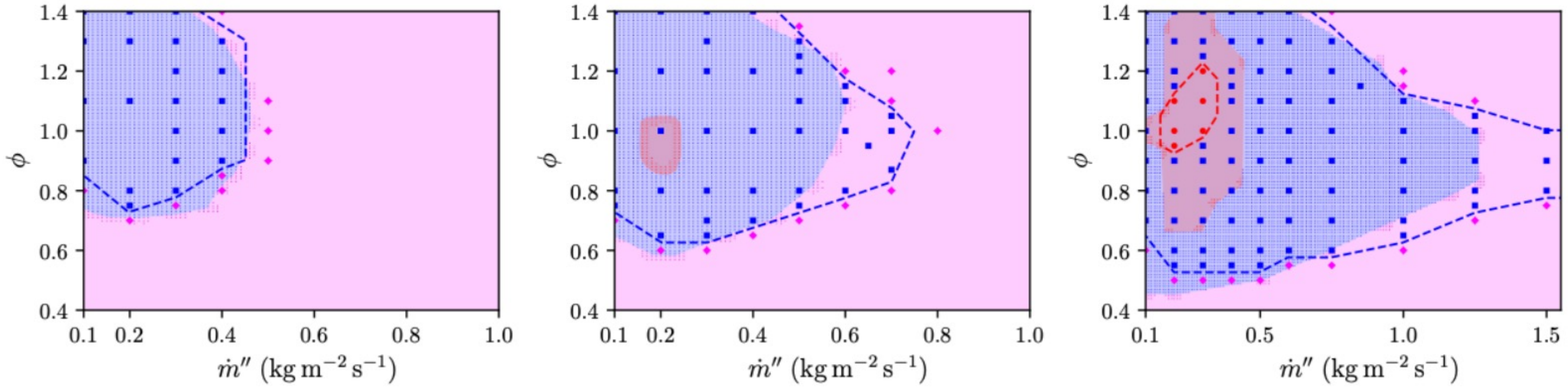
$$\rho_g \epsilon C_g \frac{\partial T_g}{\partial t} + \rho_g \epsilon C_g u \frac{\partial T_g}{\partial x} + \epsilon \sum_{i=1}^{n} \rho_{g,i} C_{g,i} V_i Y_i \frac{\partial T_g}{\partial x} + \epsilon \sum_{i=1}^{n} \dot{\omega}_i h_i W_i - \frac{\partial}{\partial x}\left(k_{g,eff} \epsilon \frac{\partial T_g}{\partial x}\right) + h_v (T_g - T_s) = 0$$

Solid temperature: $\rho_s C_s \frac{\partial T_s}{\partial t} + \frac{\partial}{\partial x}\left(\lambda_s \frac{\partial T_s}{\partial x}\right) + \frac{dq}{dx} - h_v (T_g - T_s) = 0$



1D simulation framework

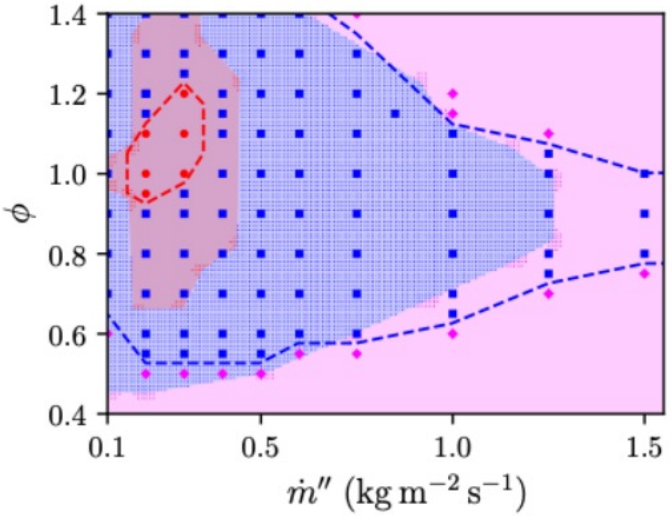
Simulations conducted using the 1D–VAS–FP framework (Table 5 and Sections 3 and 4.1).



(a) $X_{NH_3} = 100\,\%$ (b) $X_{NH_3} = 85\,\%$ (c) $X_{NH_3} = 70\,\%$

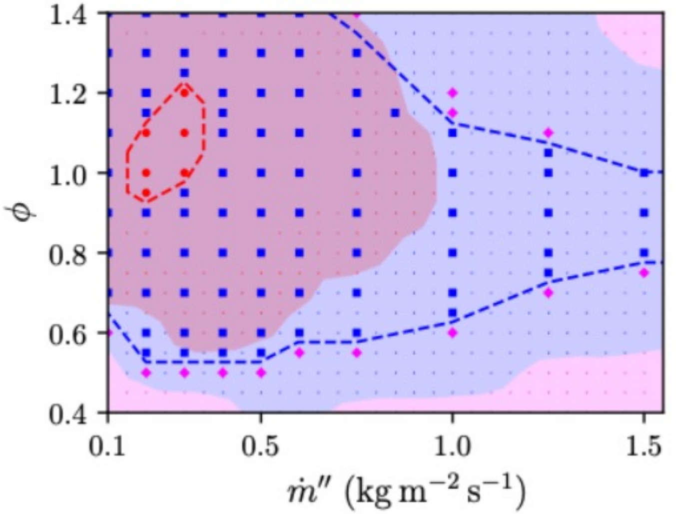
- 1D simulations can capture the experimentally determined stability limits of the burner when accurate constitutive relations are used.
- Pollutant emissions are also captured well.

1D simulation framework



(c) $X_{NH_3} = 70\,\%$

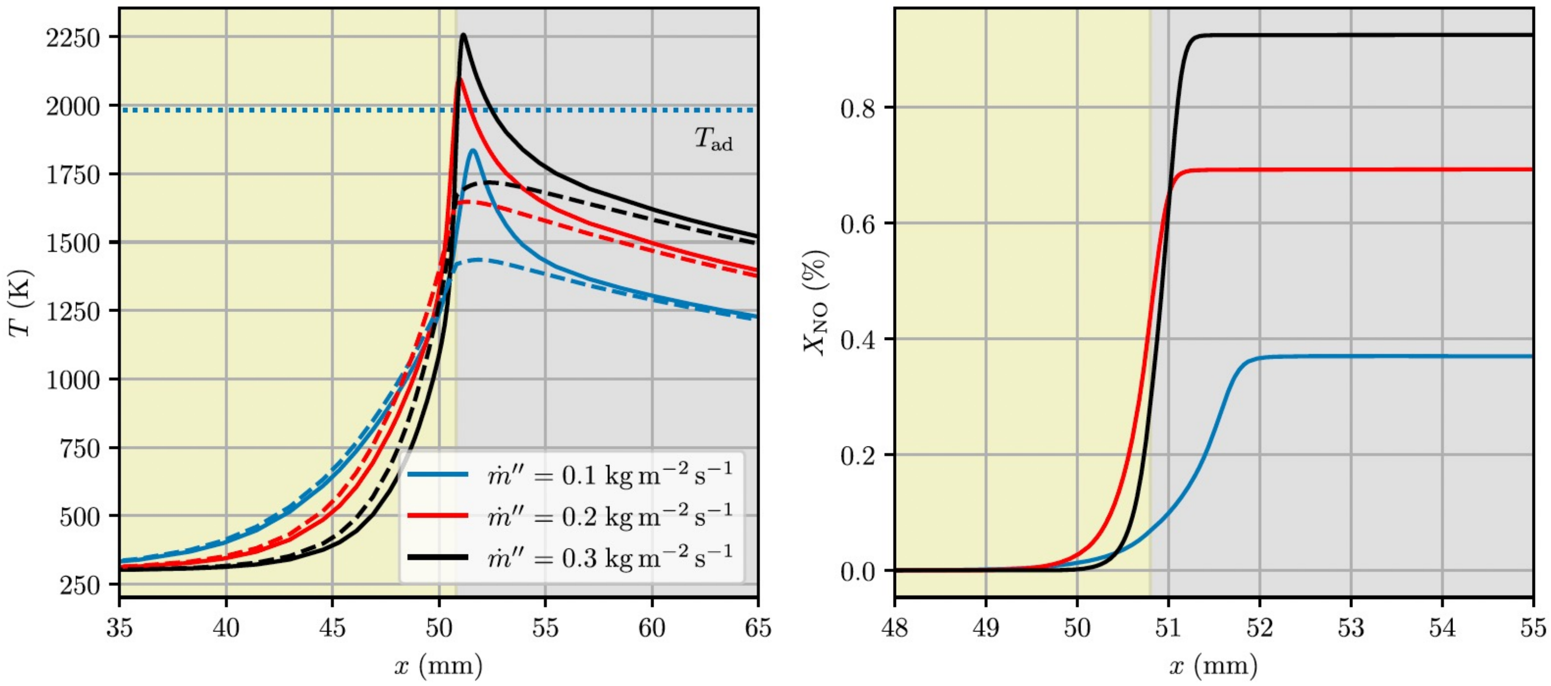
Accurate constitutive relations from processed μCT scans.



(f) $X_{NH_3} = 70\,\%$

Literature correlations for constitutive relations.

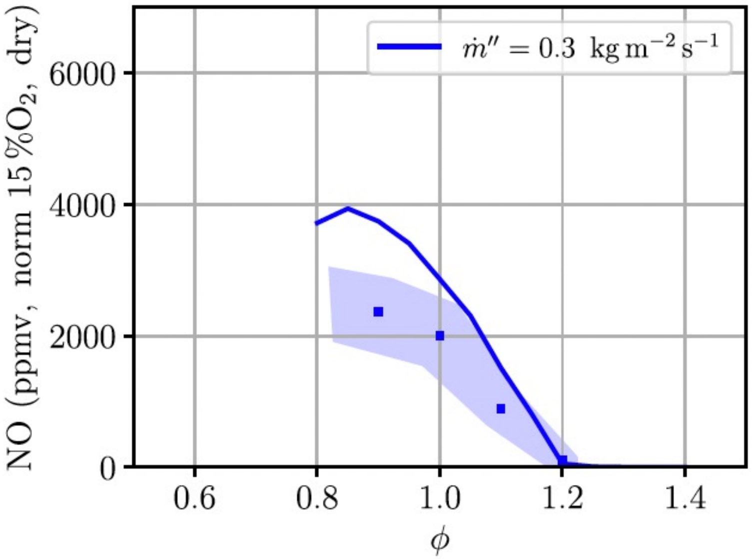
1D Simulations



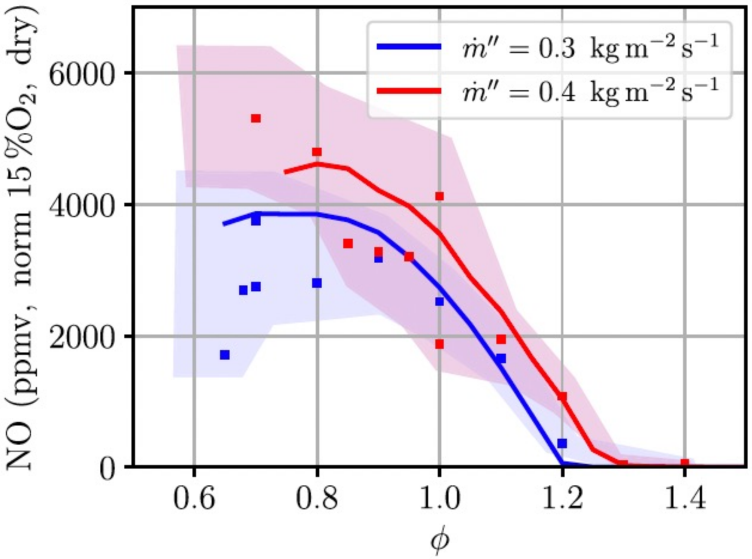
(a) Temperature

(b) NO mole fraction

1D Simulations



(a) $X_{NH_3} = 100\,\%$



(b) $X_{NH_3} = 85\,\%$

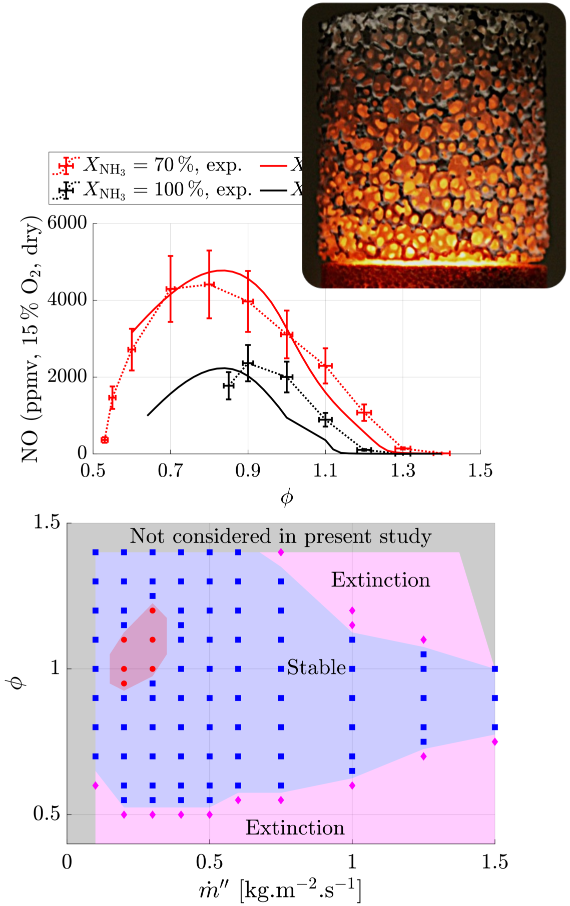
Conclusions

Demonstrated first porous media burner for pure NH_3 combustion.

Characterized NO, NH_3 and H_2 emissions:

- In rich condition: most unburnt gases in the form of unburnt H_2
- Unburnt NH_3 highly dependent on burner operating temperature

Introduced a reactor network and a 1D model with interphase heat transfer that captures emissions and stability to acceptable accuracy



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- G Vignat, T Zirwes, ER Toro, K Younes, E Boigné, P Muhunthan, L Simitz, D Trimis, M Ihme, Experimental and numerical investigation of flame stabilization and pollutant formation in matrix stabilized ammonia-hydrogen combustion, **Combustion and Flame** 250, 112642, 2023.
- D Mohaddes, C Chang , M Ihme, Thermodynamic cycle analysis of superadiabatic matrix-stabilized combustion for gas turbine engines, **Energy** 207, 118171, 2020.
- S Sobhani, D Mohaddes, E Boigne, P Muhunthan, M Ihme, Modulation of heat transfer for extended flame stabilization in porous media burners via topology gradation, **Proceedings of the Combustion Institute** 37 (4), 5697-5704, 2019.
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