Numerical analysis of ammonia dehydrogenation in porous media combustion

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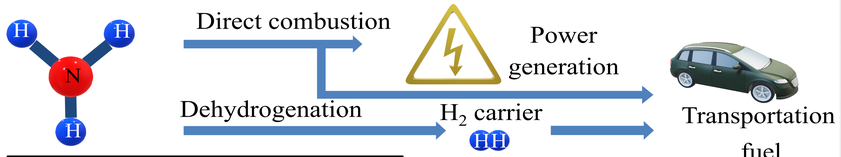
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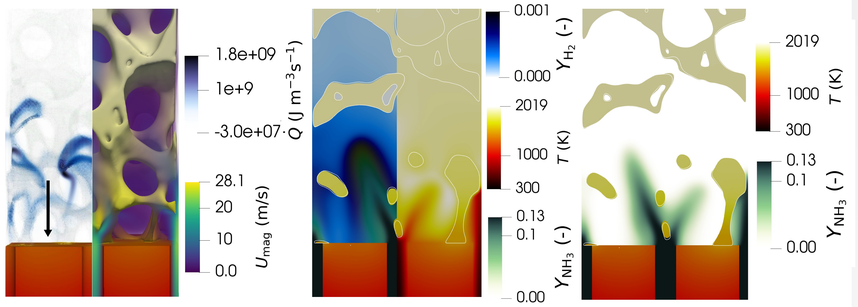
Enabling Models, Methods, Tools & Technology - Enabling concepts

Ammonia (NH_3) as a fuel



Challenges for direct combustion [1]
- Lower flame velocity → Flame instability
- High NO_x emissions and NH_3 slip

Solution → Porous media combustion (PMC) [2]



increases flame velocity

enhances NH_3 dehydrogeneation

enables complete NH_3 burnout

Modelling of porous media combustion

Volume-averaged simulations (VAS) [3]

Energy equations

$$\frac{\partial(\gamma\rho H_{tot})}{\partial t} + \nabla\cdot(\gamma\rho\vec{u}H_{tot}) = -\nabla\cdot(\gamma\vec{q}) + \gamma\frac{\partial p}{\partial t} - \gamma\sum_k(h_k^0\dot{\omega}_k) - h_v(T-T_s)$$

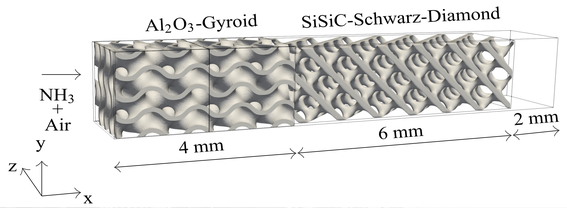
$$\vec{q} = -(0.5|\vec{u}|\boldsymbol{d_{disp}}\rho)\nabla h_s + \sum_k h_{s,k}\hat{j}_k + \frac{\lambda}{\eta c_p}\left(-\nabla h_s + \sum_k h_{s,k}\nabla Y_k\right)$$ Gas phase

$$(1-\gamma)\rho_s c_s\beta\frac{\partial T_s}{\partial t} = \nabla\cdot(\lambda_{s,eff}\nabla T_s) + \dot{Q}_{rad} + h_v(T-T_s)$$ Solid phase

Radiation modelling

$$\dot{Q}_{rad} = -\nabla\cdot\left(\frac{16\sigma T_s^3}{3\kappa}\nabla T_s\right)$$ Rosseland[4]

$$\dot{Q}_{rad} = 2\kappa(1-\omega_{rad})\sigma T_s^4 - 2\kappa(1-\omega_{rad})([\dot{q}_R^+ + \dot{q}_R^-])$$ Schuster-Schwarzschild[5]



Direct pore-level simulations (DPLS) [6]

$$\frac{\partial(\rho H_{tot})}{\partial t} + \nabla\cdot(\rho\vec{u}H_{tot}) = -\nabla\cdot\vec{q} + \frac{\partial p}{\partial t} - \sum_k h_k^{\circ}\dot{\omega}_k + \rho\vec{g}\cdot\vec{u}$$

$H_{tot} = h_s + 0.5(\vec{u}\cdot\vec{u})$

Cantera — Chemistry

Gas phase conduction

Radiation

Convection

Solid phase conduction $\nabla\cdot\left(\frac{\lambda_s}{\rho_s c_s}\nabla h\right) = 0$

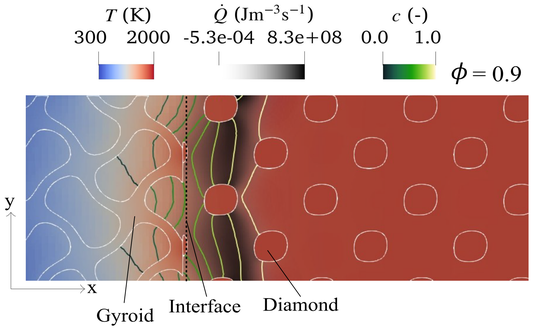
Boundary condition $\lambda\frac{dT}{d\hat{n}} = \lambda_s\frac{dT_s}{d\hat{n}} + \dot{Q}_{rad}$

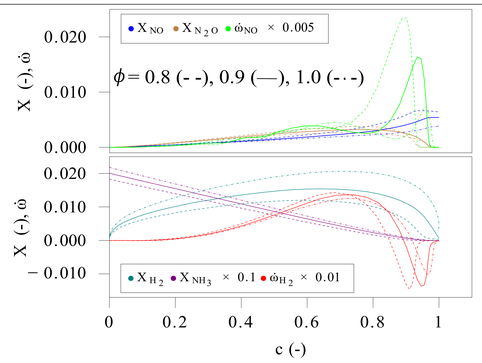
Radiation implemented as $\dot{Q}_{rad} = -\nabla\cdot(\lambda_{eff,rad}\nabla T_s)$ where $\lambda_{eff,rad}$ is extracted from VAS

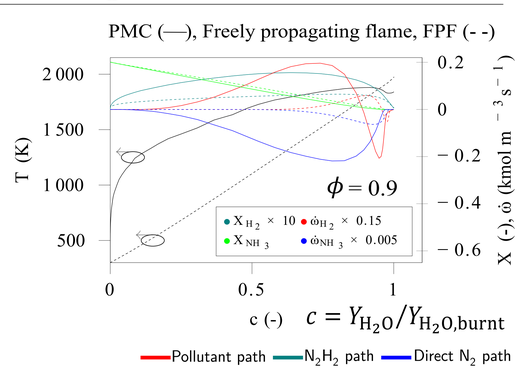
Structure	γ (-)	S_v (m^{-1})	d_p (mm)
Gyroid	0.67	6406	0.4
Diamond	0.71	3540	0.9

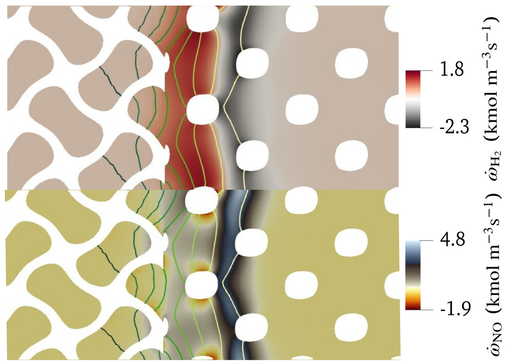
Porosity: γ; Specific surface area: S_v; Mean pore diameter: d_p

Results for burner power density P = 0.5 MWm^{-2}, and Stagni [7] mechanism

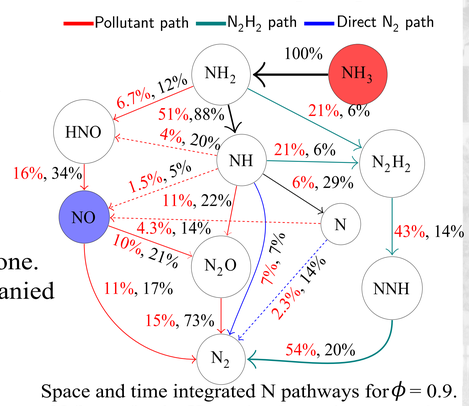








- Tailored geometries enhance NH_3 dehydrogenation.
- Flame is stabilised in the diamond zone near the interface.
- Heat recirculation is increased with $T_{s,mean,gyroid} \approx 1000$ K.
- Major H_2 production reactions are
  $NH_3 + H \rightarrow H_2 + NH_2$ (34%)
  $NH_2 + H \rightarrow H_2 + NH$ (23%)
  $N_2H_2 + H \rightarrow H_2 + NNH$ (23%)
- NO production zone coincides with the H_2 consumption zone.
- With decreasing ϕ, reducding in H_2 production is accompanied by a larger and upstream shifted NO production zone
- More active N_2H_2 path in the main reaction zone ($0<c<0.93$) leads to NO reduction.



Space and time integrated N pathways for $\phi = 0.9$. N fluxes for the H_2 production and consumption zones are shown in red and black, respectively.

Conclusions

- DPLS performed to investigate NH_3 dehydrogenation in tailored two-layer porous burner
- Operating conditions ϕ = 0.8,0.9,1.0, P = 0.51 MWm^{-2}
- NO production zone shifts upstream for decreasing ϕ
- H_2 production zone extends to higher c values for increasing ϕ
- Pollutant formation NO_x and N_2O closely related to NH_3 dehydrogenation
- N_2O fully consumed by the end of combustion
- More active N_2H_2 path increases H_2 production and simulateneously reduces NO production
- Selected material and geometrical properties enhance the heat recirculation and a 25% reduction in NO production is observed for PMC as compared to FPF
- Augmenting the solid heat conductivity in DPLS with $\lambda_{eff,rad}$ leads to a 4% increase in average gas temperature upstream of the flame front

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