6th Two-Day Meeting on Propulsion Simulations Using OpenFOAM Technology

Combustion models for hydrogen and ammonia operating under premixed and diffusive dual-fuel combustion modes

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Acknowledgments

POLITECNICO
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- Andrea Schirru

UNSW SYDNEY

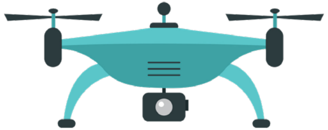
- P. Rorimpandey, Q. Chan, S. Kook, E. Hawkes (UNSW)
- S. Reggeti, W. Northrop (UNM)

Future of CI Engines

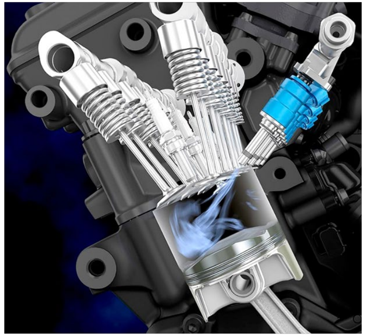
- Efficiency increase
- Reduction of emissions
- New applications



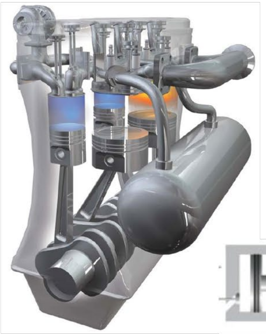
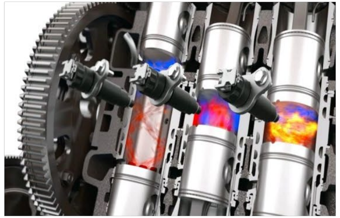
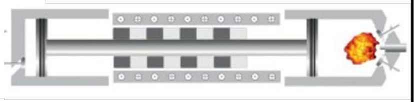


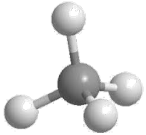
Hydrogen engines

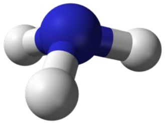
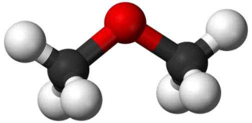
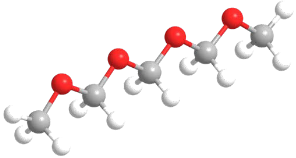



New engine concepts

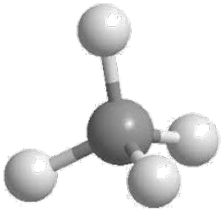




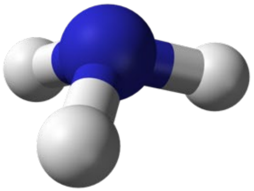
Alternative fuels

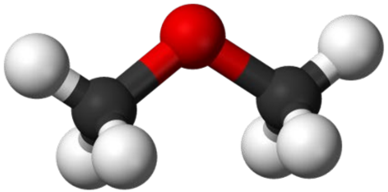


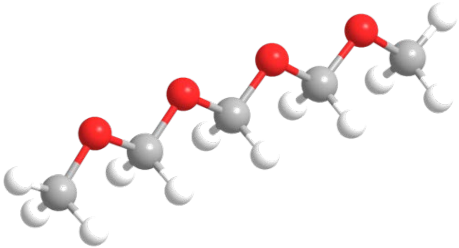




Alternative fuels









- H_2 and NH_3 potential: maritime/long-haul transport, off-road, power-generation
- Efficient conversion of H_2 and NH_3 is crucial: conventional combustion systems are not completely suitable (knock, ON, backfire, flame speed)
- **Dual-fuel combustion**: an interesting solution to burn efficiently low-carbon fuels under different modes.

New engines... which models?

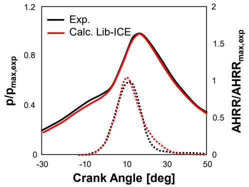
- Including the fuel-to-fuel interaction: kinetics, mixing
- Computationally efficient

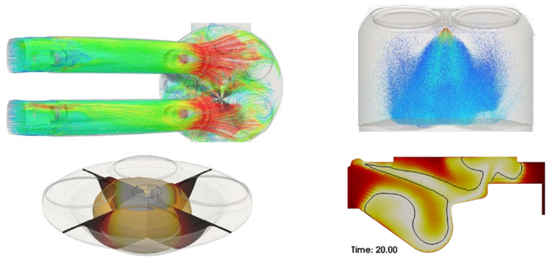
Modeling methodology and validation:

- **H2DDI** : Hydrogen-Diesel Direct Injection combustion
- **Ammonia**
  - Spark-ignition with H_2 active prechamber

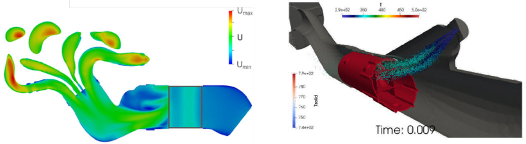
Lib-ICE : engines (and more...) in OpenFOAM

Internal combustion engines

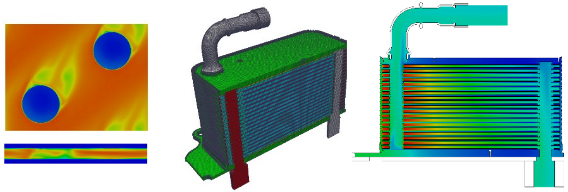




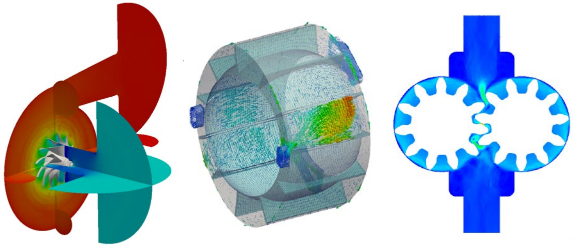
After treatment systems



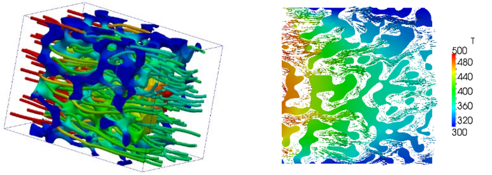
Thermal management



Fluid machines

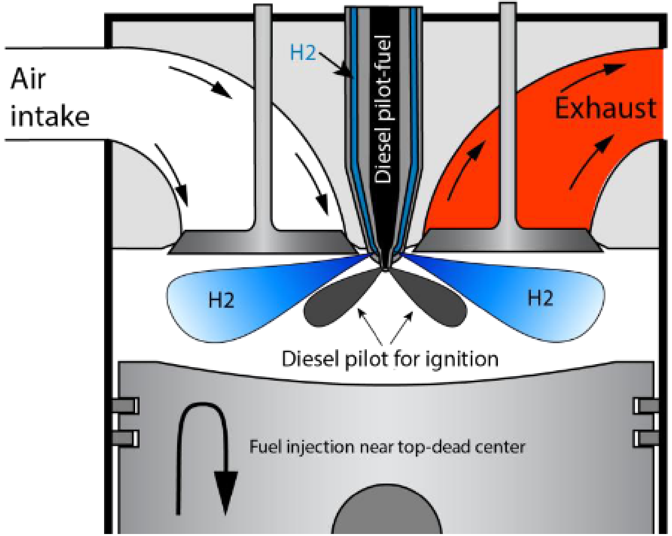


Porous media



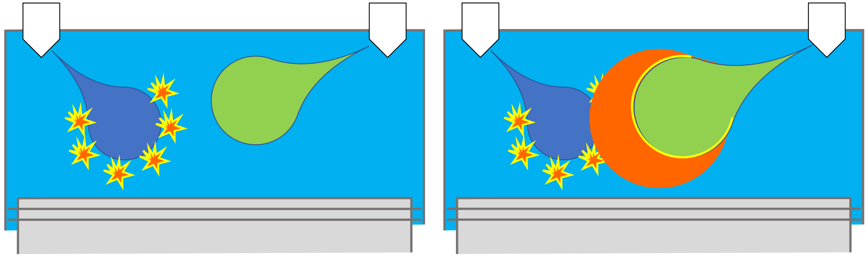
H_2 Diesel Dual-fuel direct injection (H2DDI)

High-pressure (100-600bar) direct-inj.
Pilot-fuel or pre-chamber ignition



Key challenges: High-pressure pump, NOx, fuel compression energy

Source Sandia



⇨ **Best efficiency, power density and transient response.**

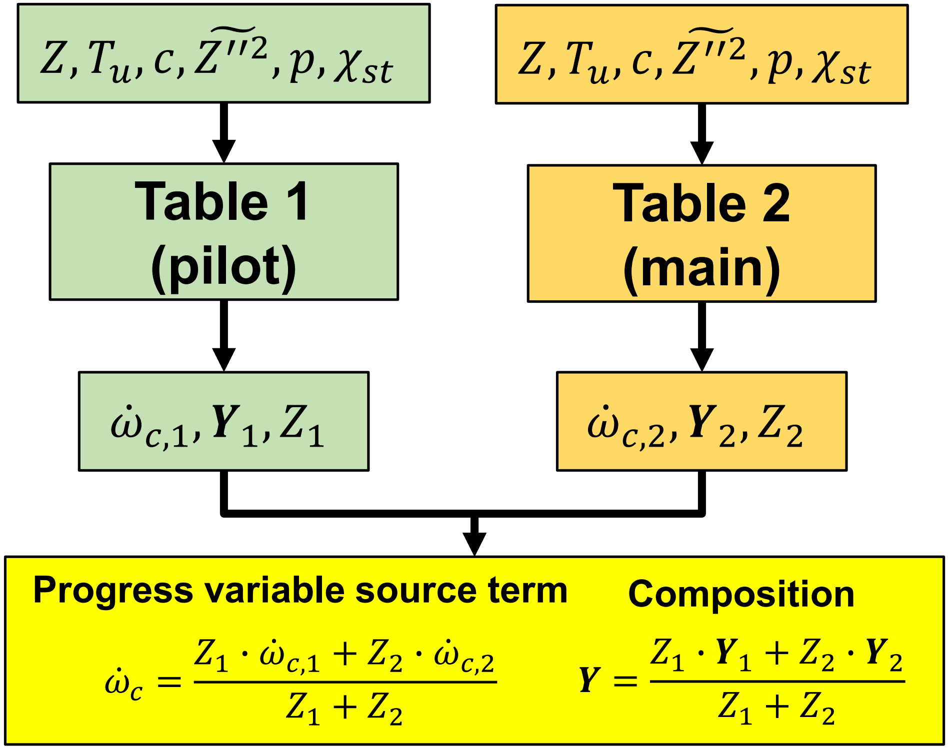
Modeling challenges

- Ignition of the pilot fuel and main jet;
- Effect of injection strategy (timing and combination of pilot + main) producing different combustion modes;

H2DDI combustion model : kinetics – flame structure

Pilot fuel ignited before interacting with the main jet

- Combustion model: tabulated kinetics (FGM)
- Separated tables for Fuel 1 (pilot) and Fuel 2 (main)
- Ignition via progress variable convection and diffusion
- Tabulated flame structures:
  - Fuel 1 (pilot) : diffusion flamelet
  - Fuel 2 (main): homogeneous constant-pressure reactor



Presumed PDF (PDF + FGM)

$$\psi = (Y_i, c, \dot{\omega}_c, h, h_u)$$

$$\tilde{\psi}_\alpha = \int_0^1 \int_Z \psi_\alpha(Z)\beta\left(\tilde{Z}, \widetilde{Z''^2}\right)\delta(c)dzdc$$

- Mixture fraction: β distribution
- Progress variable: δ distribution

Eulerian Monte-Carlo Fields (EMCF+PDF)

- **Stochastic fields $\xi^{(j)}$**

$$\xi^{(j)} = \left(Y_i^{(j)}, c^{(j)}, \dot{\omega}_c^{(j)}\right) \rightarrow \tilde{\psi}_a = \frac{1}{N_s}\sum_{j=1}^{N_s} \xi_\alpha^{(j)}$$

- **Stochastic differential equations**

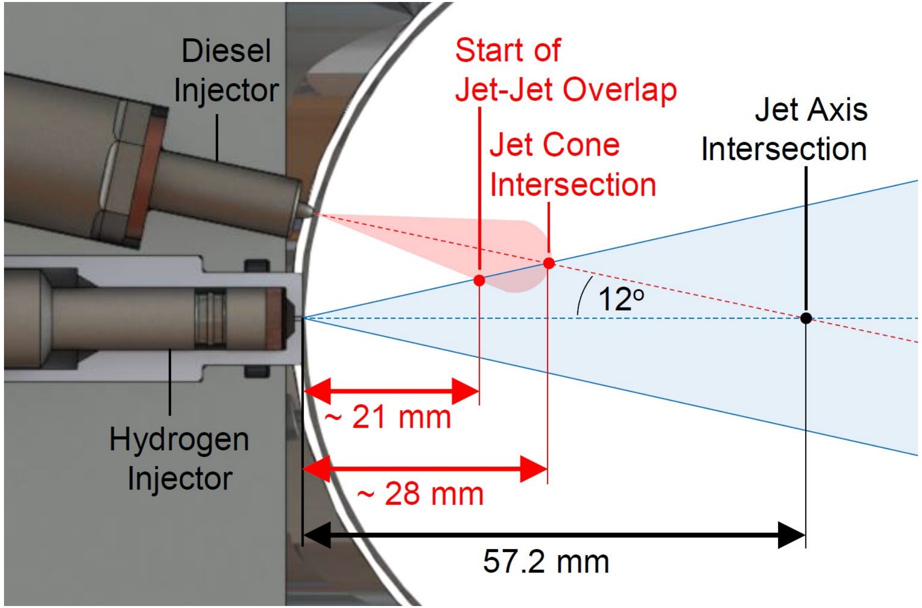
$$d\bar{\rho}\xi_a^{(j)} = -\frac{\partial \bar{\rho}\tilde{u}_i \xi_a^{(j)}}{\partial x_i} dt + \frac{\partial}{\partial x_i}\left[(\Gamma + \Gamma_t)\frac{\partial \xi_a^{(j)}}{\partial x_i}\right] dt$$

$$+\frac{1}{2}\bar{\rho}C_\phi \frac{\varepsilon}{k}\left(\xi_a^{(j)} - \tilde{\psi}_a\right) dt$$ → Mixing

$$+\bar{\rho}\sqrt{2(\Gamma + \Gamma_t)}\frac{\partial \xi_a^{(j)}}{\partial x_i} dW_i$$ → Stochastic term

$$+\dot{S}_{spray}dt + \dot{S}_{FGM}dt + \dot{S}_p dt$$

H2DDI combustion : UNSW CVCC



T_{amb} = 890 K, p_{amb} = 5.2 MPa, O_2% = 21%		
Fuel	**nC_7H_{16}**	**H_2**
Nozzle diameter [mm]	0.105	0.58
Fuel pressure [MPa]	70	20
Injection duration [ms]	0.7	3.3
Mass injected [mg]	0.99	5.28
Energy share [%]	6	94

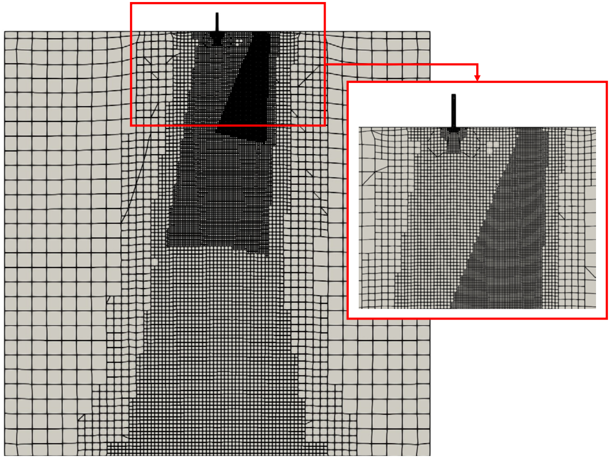
		Dwell time		**Injection strategy**
		Pilot	Main	
1	H-0.07-ms-D	0.07 ms	-	Main-Pilot
2	H-2.07-ms-D	2.07 ms	-	Main-Pilot
3	D-1.93-ms-H	-	1.93 ms	Pilot-Main

Combustion analysis:

- Vessel pressure measurement
- High-speed Schlieren

H2DDI combustion : case setup

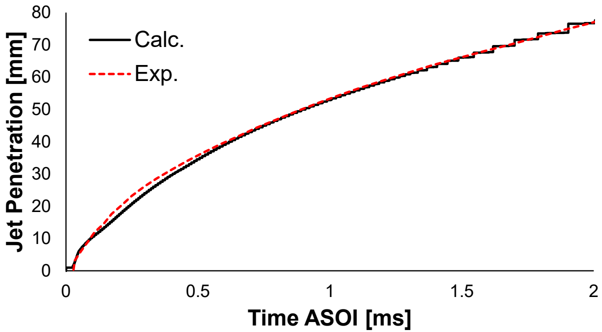
Computational mesh



- Full vessel geometry;
- 450’000 cells;
- Local refinements: jets evolution and interactions

CFD sub-models

- Turbulence: $k - \varepsilon\ (C_1 = 1.5)$;
- Spray model: lagrangian
  - Injection profile: ECN;
  - Breakup model: KHRT;
- Hydrogen jet: flow rate profile tuned to match the exp. jet penetration



Combustion model

Tabulation

- Skeletal nC_7H_{16} mechanism
- Ranges:
  - T_{ox} = 700-1200 K
  - p = 4 – 7 MPa
  - ϕ = 0.05 – 6
  - χ_{st} = 1 – 200 s^{-1}
- Flamelet table nC_7H_{16}: Lib-ICE utility + DLBFoam;
- Homogeneous reactor H_2 table: OpenSMOKE utility.

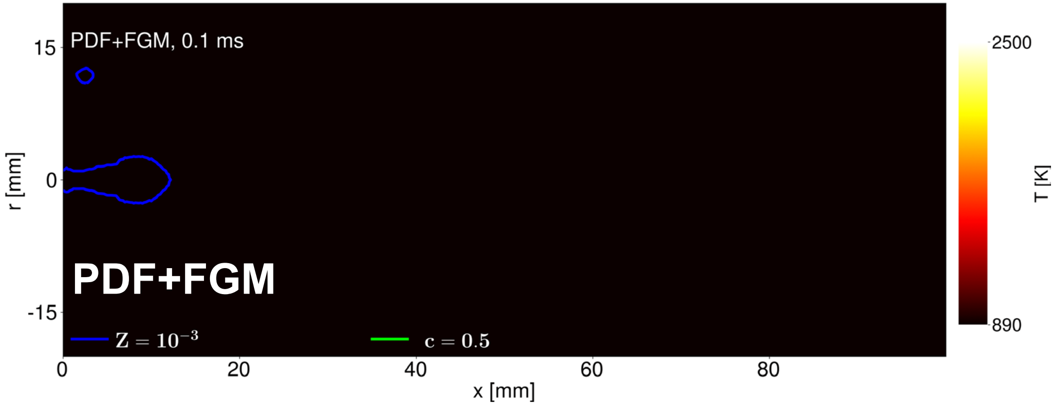
EMCF

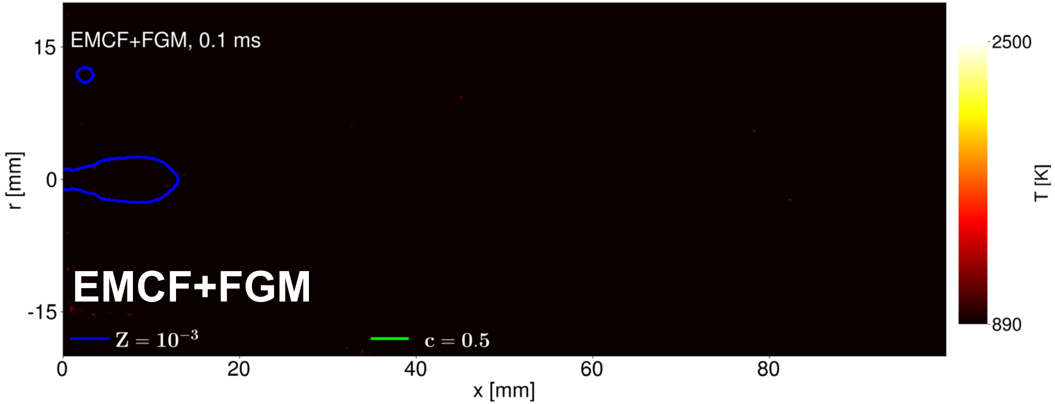
- 16 stochastic fields

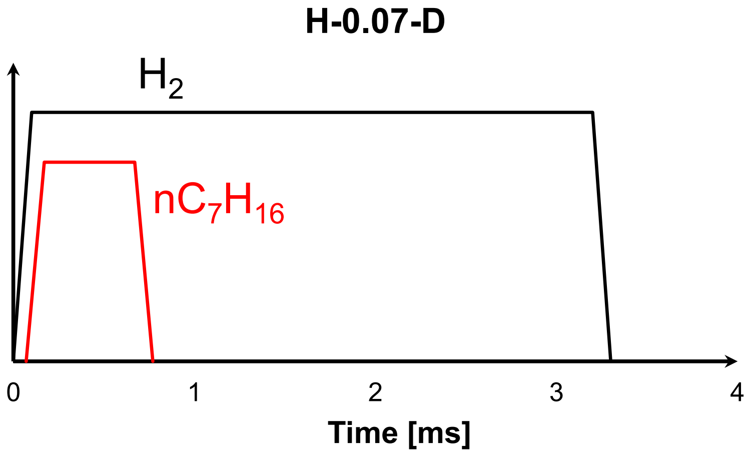
Stagni et al., *Skeletal mechanism reduction through species-targeted sensitivity analysis*, Combust. Flame
Morev I., et al., *Fast reactive flow simulations using analytical Jacobian and dynamic load balancing in OpenFOAM* (2022) Phys. Fluids
A. Cuoci, et al., *OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms* (2015) Comput. Phys. Comm.

Acknowledgments: P. Rorimpandey, Q. Chan, S. Kook, E. Hawkes (UNSW)

H2DDI combustion : H-0.07-ms-D







- nC_7H_{16} and H_2 burning in a diffusive mode;

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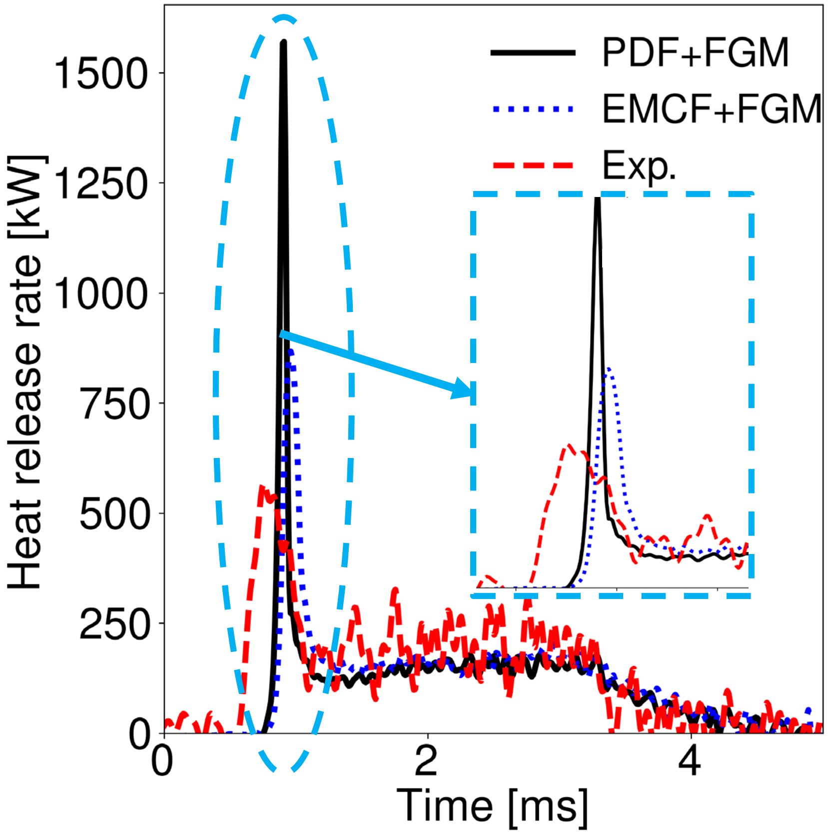
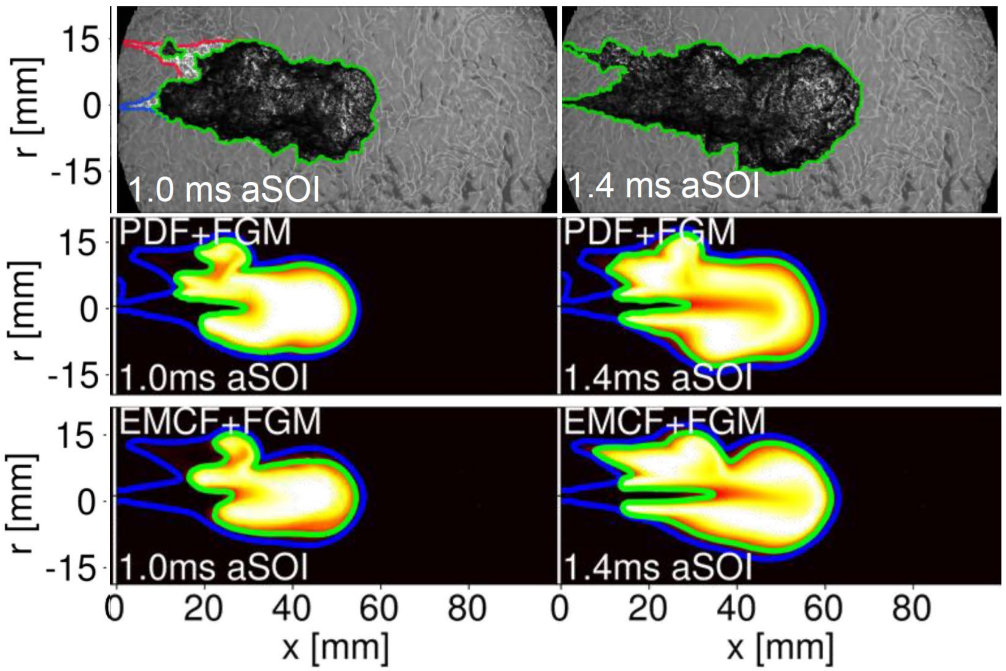
H2DDI combustion : H-0.07-ms-D





- Overestimated nC_7H_{16} ignition delay
- Diffusive mode burning correctly estimated
- EMCF+FGM : better prediction of the flame morphology

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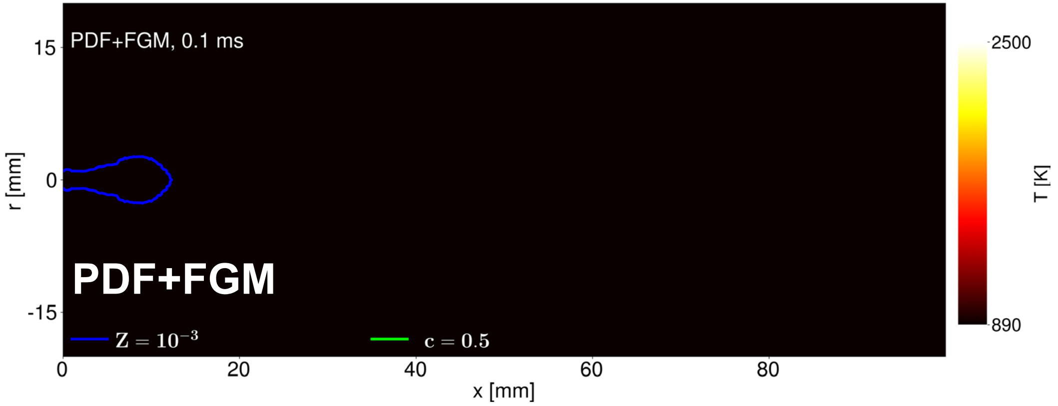
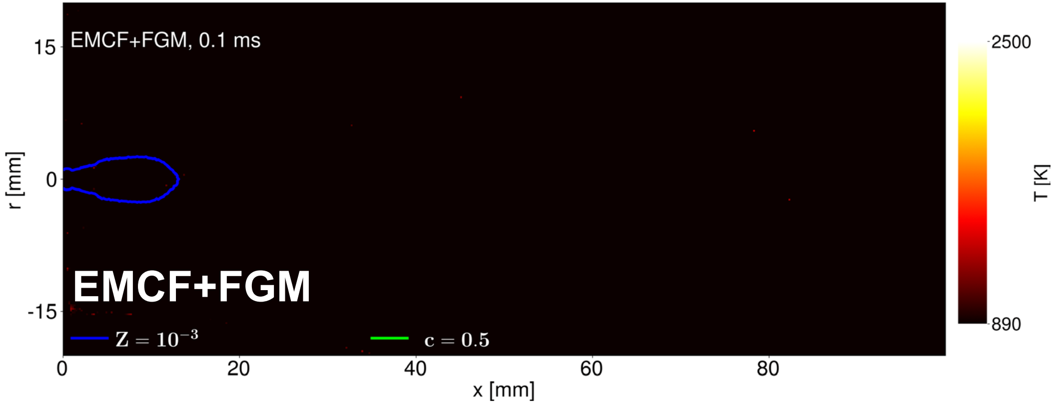
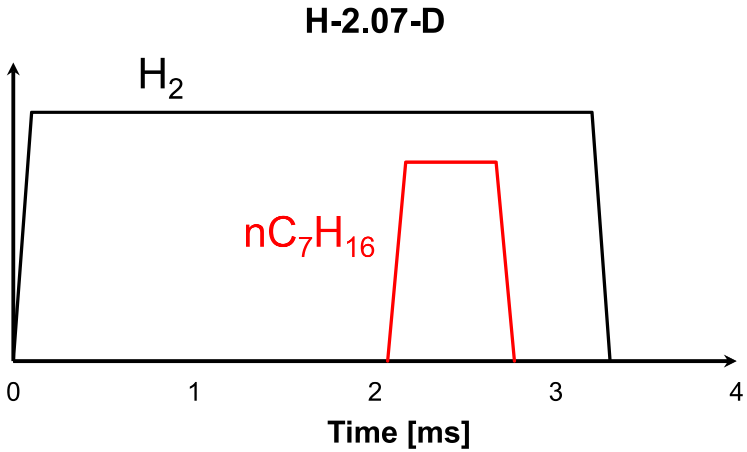
H2DDI combustion : H-2.07-ms-D







- Pilot nC_7H_{16} ignition produces H_2 partially premixed combustion

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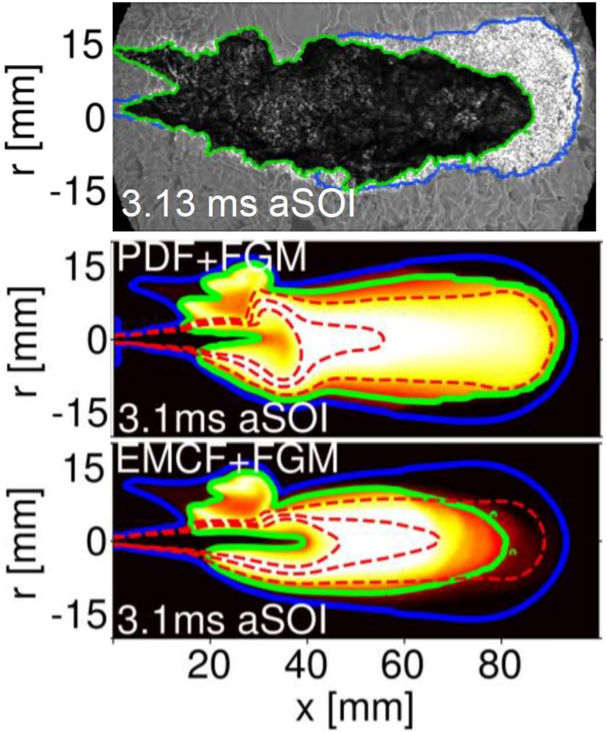
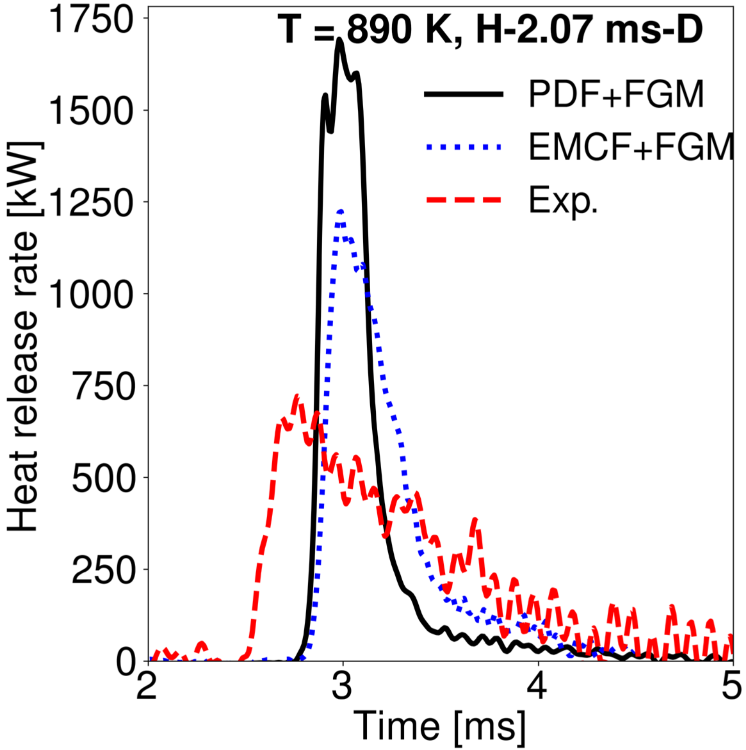
H2DDI combustion : H-2.07-ms-D

H_2 partially-premixed combustion



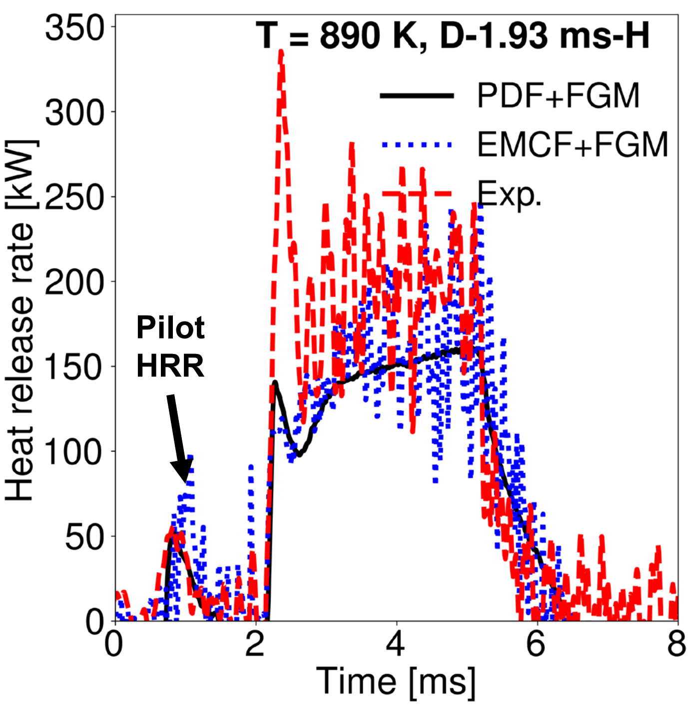


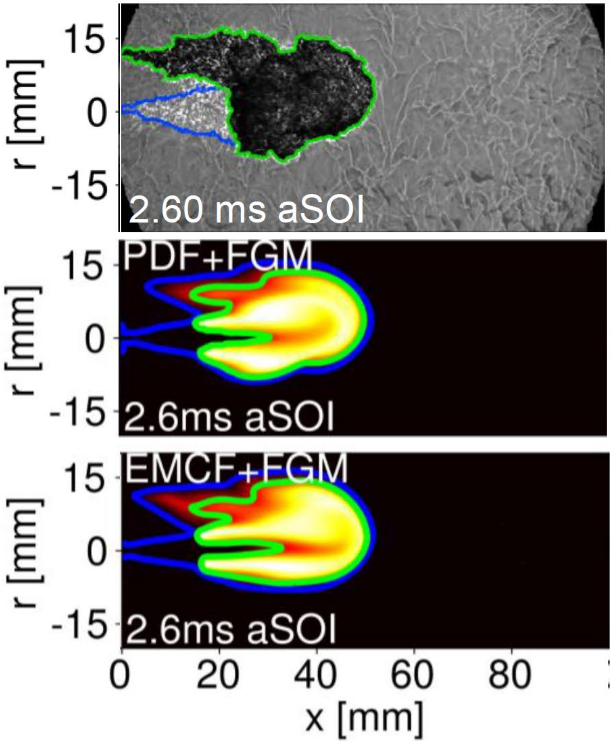
- EMCF+FGM : better estimation of AHRR and combustion duration;
- Results still affected by overestimated nC_7H_{16} ignition delay;
- “Conventional” fuel kinetics even more important in dual-fuel combustion simulations.

Acknowledgments: P. Rorimpandey, Q. Chan, S. Kook, E. Hawkes (UNSW)

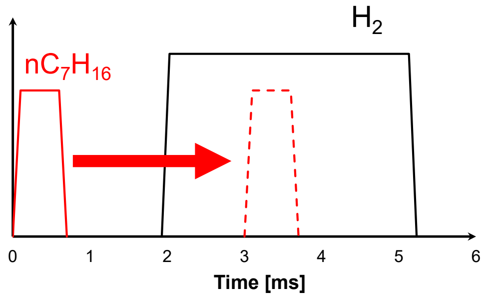
H2DDI combustion : D-1.93-ms-H

H_2 injected 1 ms after nC_7H_{16} ignition





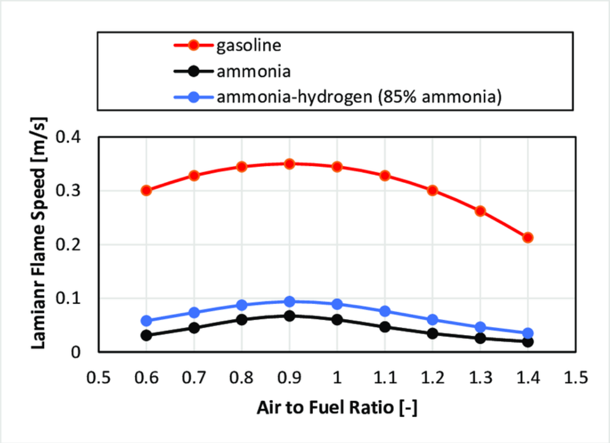
Diffusive combustion correctly estimated rather well in a wide range of nC_7H_{16} SOI



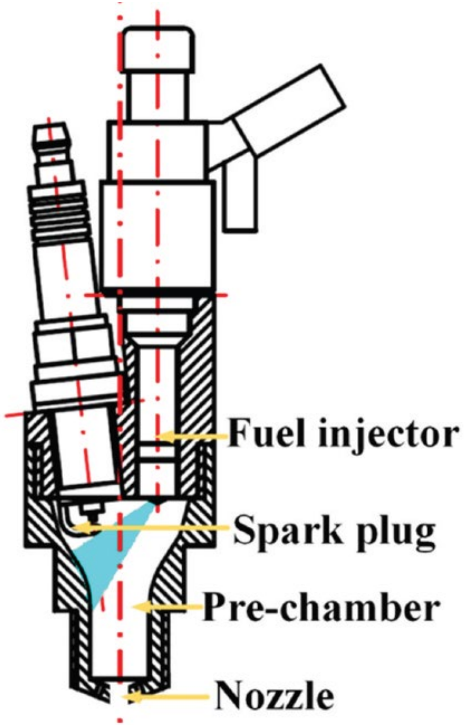
Acknowledgments: P. Rorimpandey, Q. Chan, S. Kook, E. Hawkes (UNSW)

NH_3 premixed combustion in IC engines

- Ammonia is an ideal candidate as future energy carrier;
- Limitation: low flame speed, high ignition energy.



H_2-fueled active prechamber in ammonia SI engines



Solution to compensate the low NH_3 laminar flame speed:

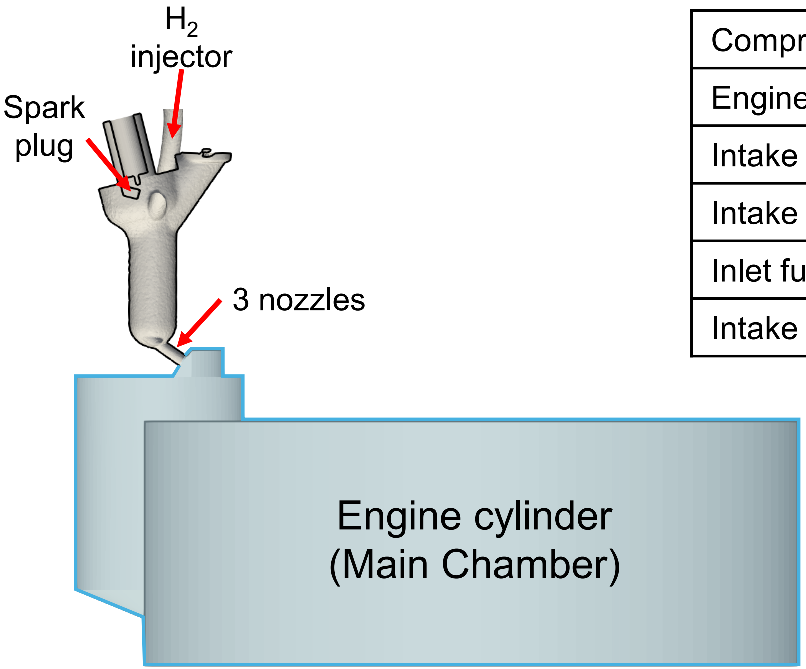
- Volumetric ignition concept (turbulent jet ignition)
- High H_2 reactivity

Effective with reduced amount of H_2/NH_3 ratio:

- Possibility to use an on-board fuel-reformer

NH_3 spark-ignition engine with active H_2 prechamber

CFR Engine with side-mounted active prechamber



Compression ratio	16:1
Engine speed [rpm]	900
Intake pressure [bar]	0.93
Intake temperature [°C]	60
Inlet fuel	100% NH_3
Intake Equivalence Ratio [-]	1

Pre-chamber fuel	H_2
Injection Pressure [bar]	38
Fuel temperature [°C]	37
Intake temperature [°C]	60

Effects of H_2 injection strategy

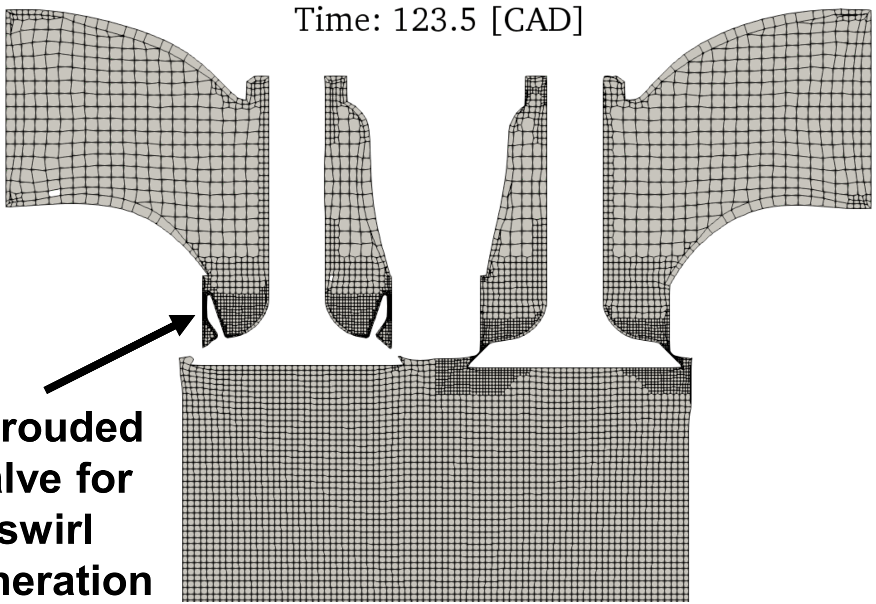
	Inection duration [ms]	SOI [CAD BTDC]	SA [CAD BTDC]	H_2/NH_3 ER [MJ_{H2}/MJ_{NH3}]
Baseline	**1**	**70**	**20**	**1.92%**
Delayed	**1**	30	20	1.99%
Double	2	**70**	20	3.48%

Acknowledgments: S. Reggeti, W. Northrop (UMN)

NH_3 spark-ignition engine with active H_2 prechamber

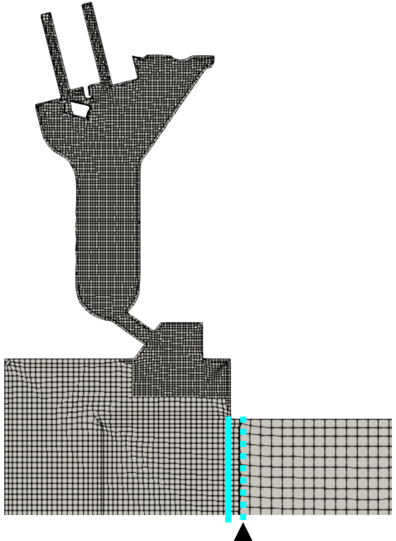
Computational mesh details

Mesh motion



Shrouded valve for swirl generation

Pre-chamber

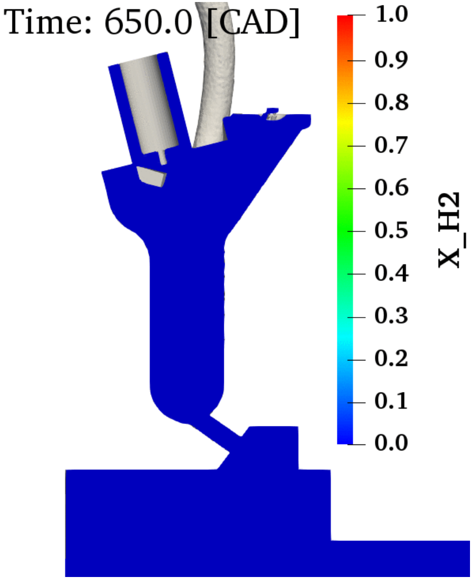


ACMI connecting cylinder and pre-chamber volume

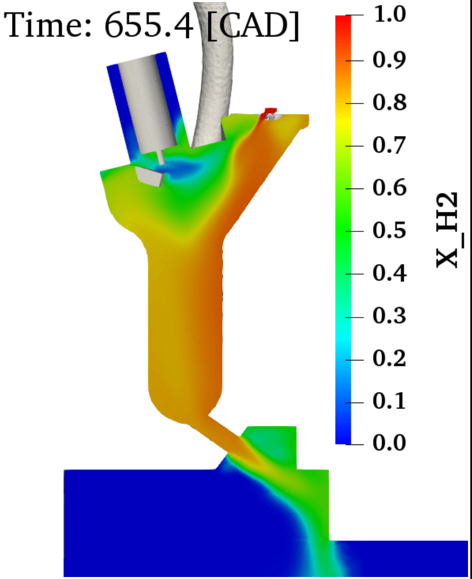
NH_3 spark-ignition engine with active H_2 prechamber

Baseline (SOI = 650)

Injection



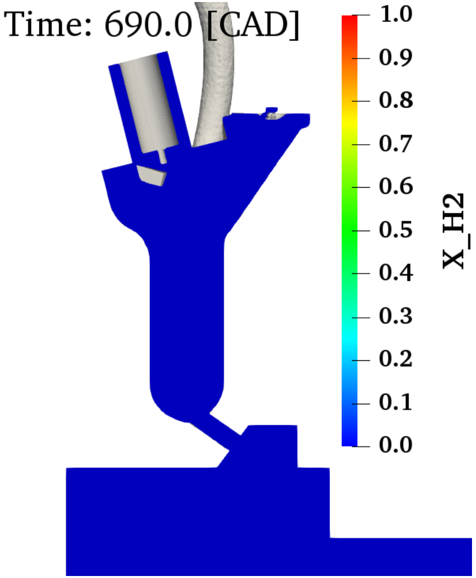
Post-injection



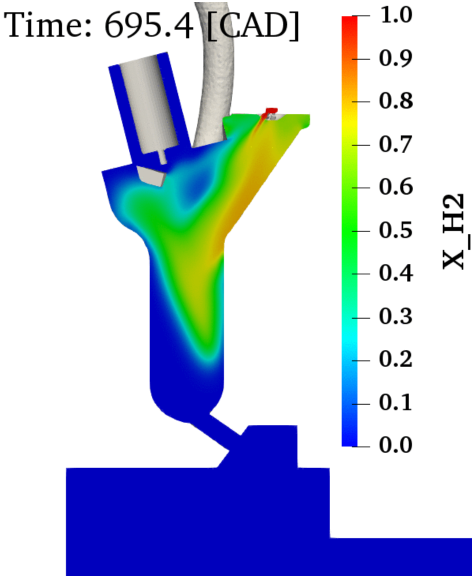
H_2 leaves the prechamber during injection

Delayed (SOI = 690)

Injection

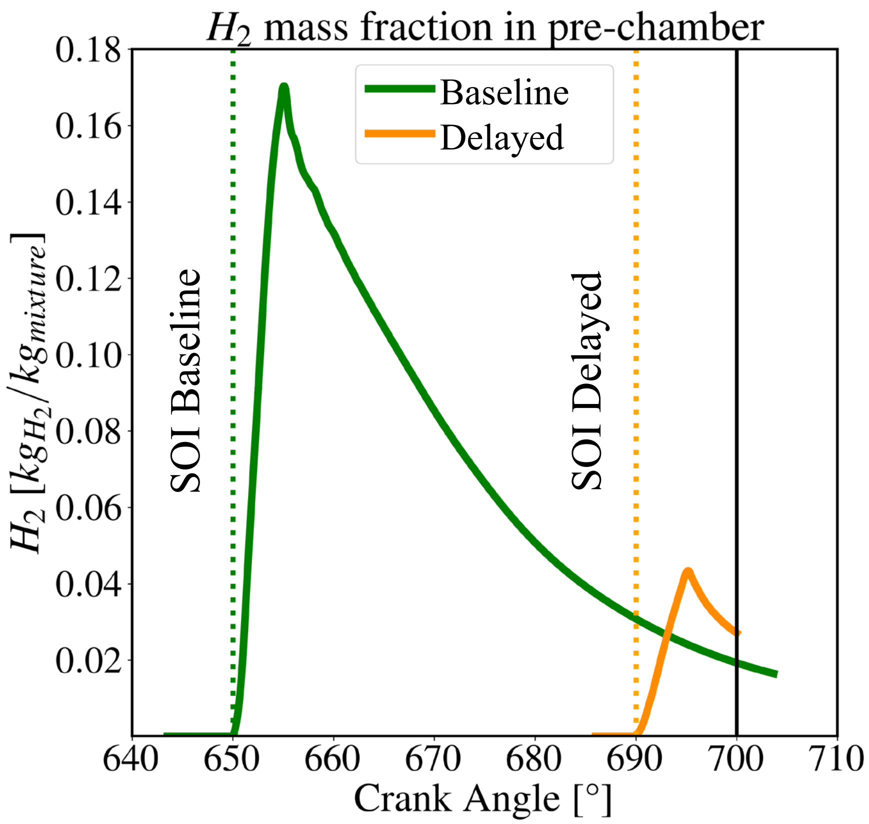


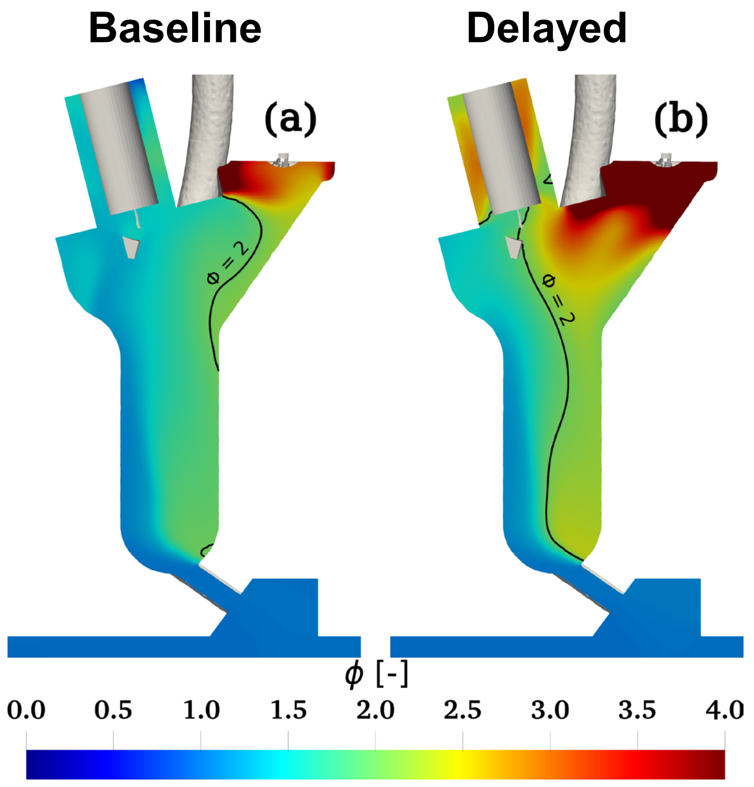
Post-injection



H_2 remains in the prechamber

NH_3 spark-ignition engine with active H_2 prechamber





Spark-ignition flame-area combustion model

Regress variable transport equation

$$\frac{\partial \rho b}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} b) - \nabla \cdot (\mu_t \nabla b) = \underbrace{\rho_u S_u \Xi |\nabla b|}_{\text{Turbulent flame speed}} + \underbrace{\dot{\omega}_{ign}}_{\text{Ignition}}$$

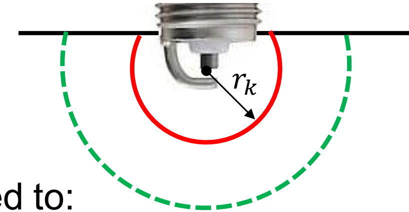
- b : unburned gas mass fraction
- Ξ : flame wrinkle factor (S_t/S_u)
- S_u : laminar flame speed
- $\dot{\omega}_{ign}$: ignition source term

Ignition: deposition model

$$\dot{\omega}_{ign} = \frac{C_s \rho_u b}{\Delta t_{ign}}$$

- C_s : user-defined
- Δt_{ign} ignition duration
- ρ_u is the unburned gas density

Turbulent combustion



$$S_t = S_u \Xi$$

$$\Xi = 1 + f \cdot (\Xi_{eq} - 1)$$

Gulder: $\Xi_{eq} = 1 + C \cdot \sqrt{\frac{u'}{S_u}} R_\eta$

Transition factor f related to:
- turbulence intensity u'
- turbulent integral length L_i
- flame radius r_k, estimated from a 0-D model
- flame stretch factor I:
  - Laminar $r_k < C_{Tay} \cdot \lambda$
  - Turbulent $r_k > C_{Tay} \cdot \lambda$

Acknowledgments: S. Reggeti, W. Northrop (UMN)

Laminar flame speed of hydrogen-ammonia mixtures

Correlation for H_2-NH_3 mixtures

$$S_u = S_{u0}(\phi)\left(\frac{T_u}{T_0}\right)^m\left(\frac{p}{p_0}\right)^n$$

- Parameters m and n are ϕ-dependent;
- $S_{u0}(\phi)$ limited validity ($\phi < 1.5$), extension required

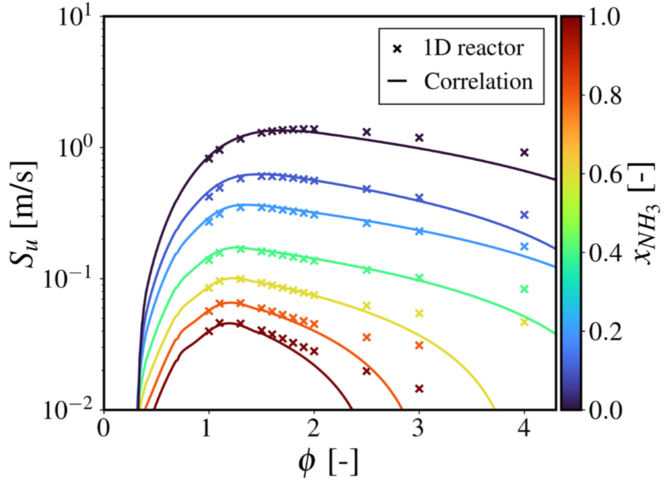
V. Pessina et al., *Laminar flame speed correlations of ammonia/hydrogen mixtures at high pressure and temperature for combustion modeling applications* (2022) Int. J. Hydrogen Energ

Extension for rich mixtures ($\phi > 1.5$)

S_{u0} correlation for $\phi > 1.5$:

$$S_{u0} = \sum_{i=0}^{5} a_i(x_{NH_3}, \phi)\phi^i$$

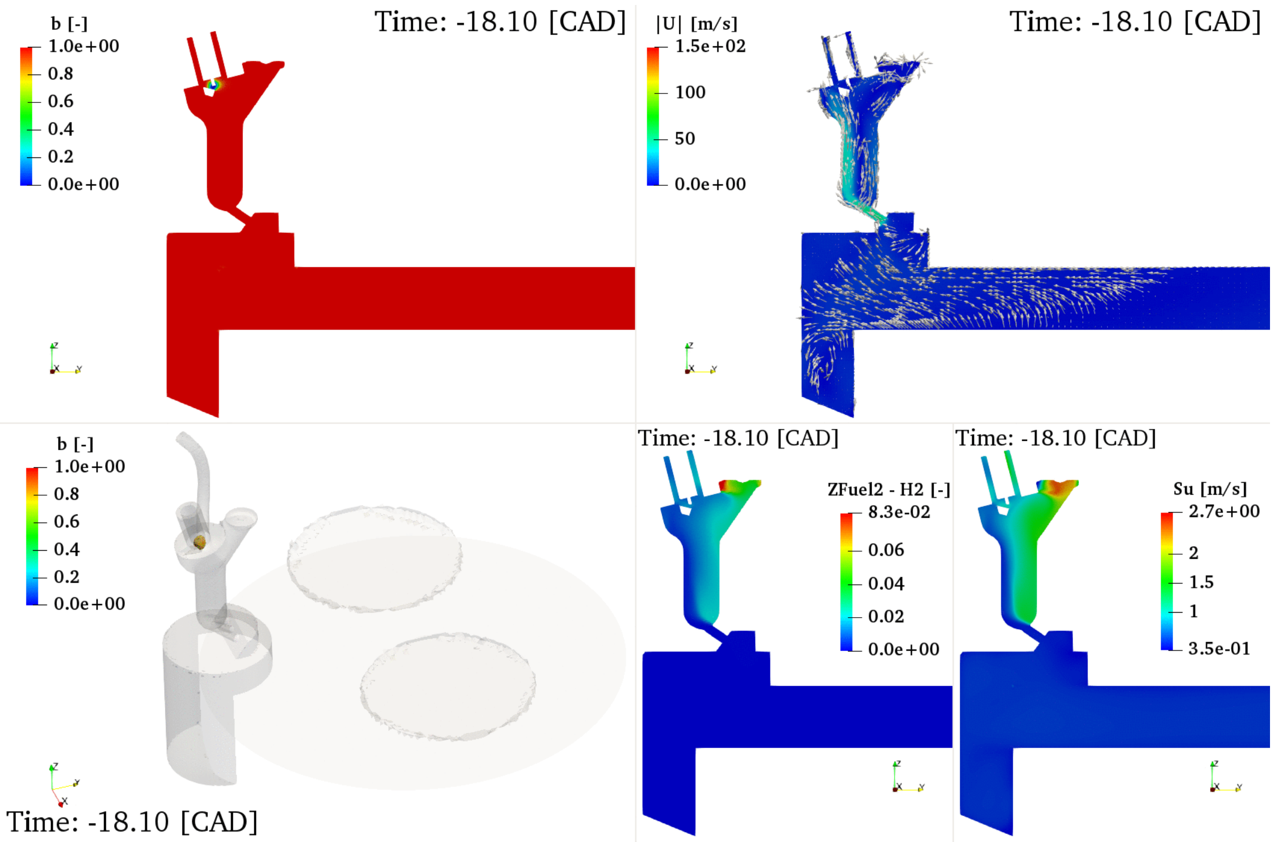
- Verified with 1D laminar flame speed simulations of NH_3-H_2 mixtures



Ravi et al., *Laminar flame speed correlations for pure-hydrogen and high-hydrogen content syngas blends with various diluents* (2012) Int. J. Hydrogen Energ.

Stagni A., et al, *Low- and intermediate temperature ammonia/hydrogen oxidation in a flow reactor: Experiments and a wide-range kinetic modeling* (2023) Chem. Eng. J S.

NH_3 spark-ignition engine with active H_2 prechamber



Baseline

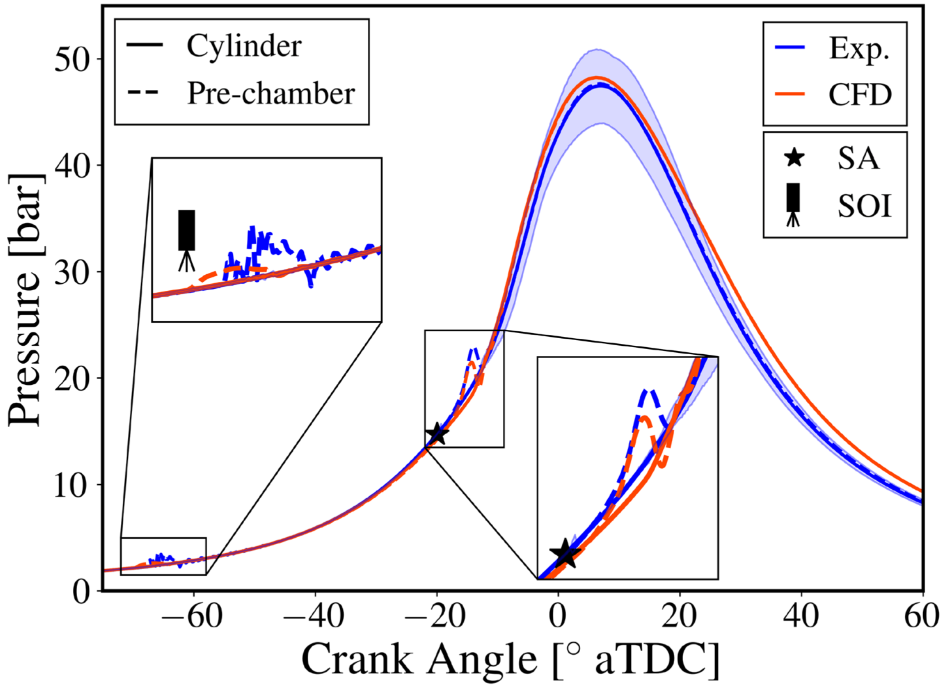
Four combustion phases

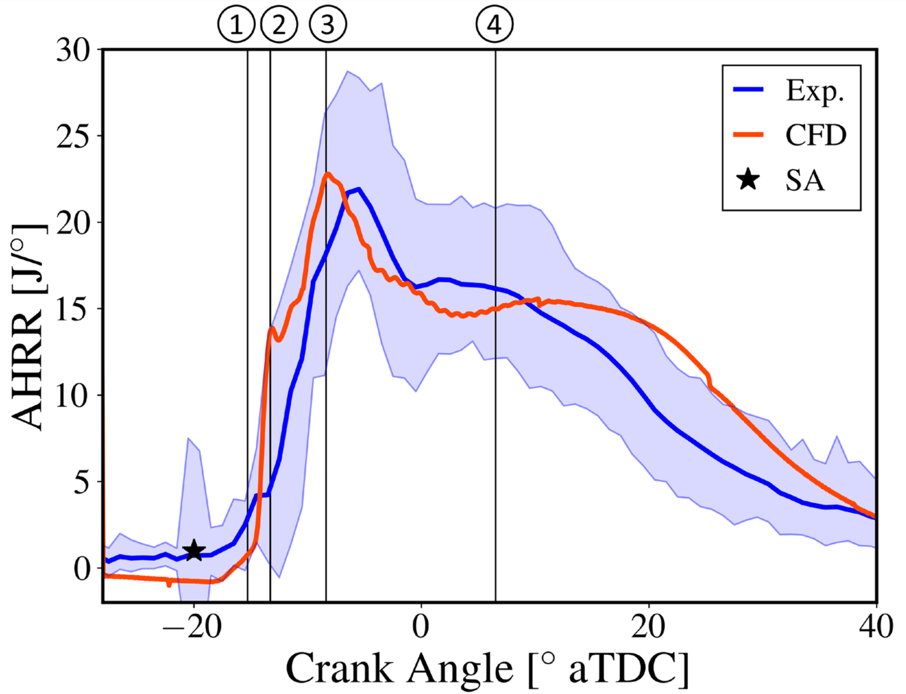
1. Pre-Chamber combustion
2. Jet-ignition in the main chamber
3. Fully-turbulent flame propagation (cylinder + side housing)
4. Flame propagation in the cylinder

Acknowledgments: S. Reggeti, W. Northrop (UMN)

NH_3 spark-ignition engine with active H_2 prechamber

Baseline condition





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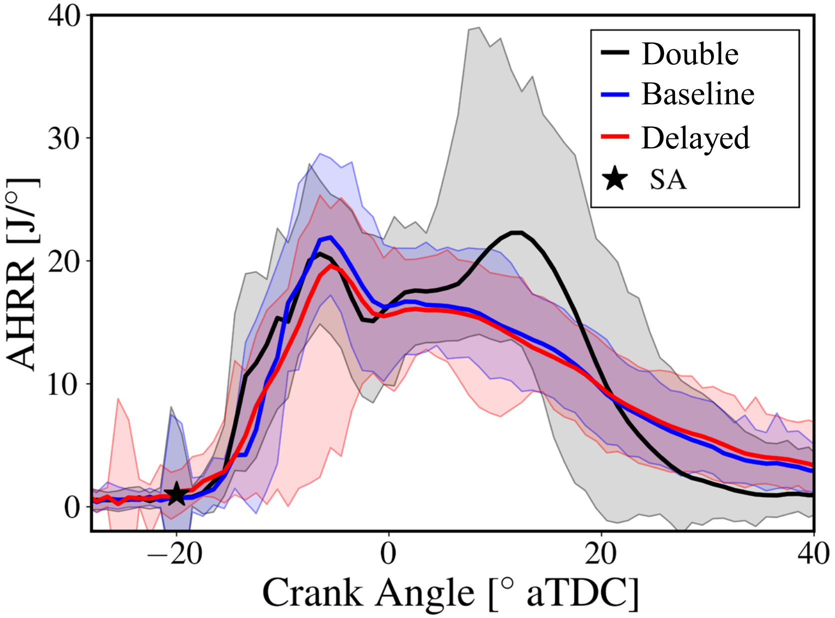
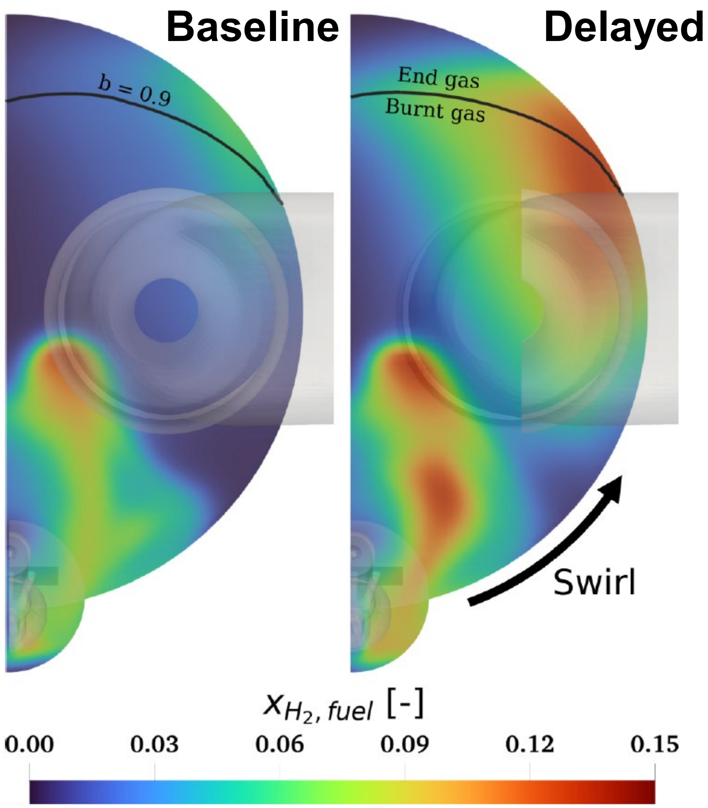
NH_3 spark-ignition engine with active H_2 prechamber





- **Double**: in-cylinder leaked H_2 + high fresh charge temperature produce fresh charge auto-ignition
  - ⇨ Transition to «SACI» combustion;
- Need to include unburned mixture kinetics to predict such process.

Acknowledgments: S. Reggeti, W. Northrop (UMN)

Conclusions

Dual fuel combustion with H_2 and NH_3 - *New engines... New models!*

⇨ **H_2-Diesel Direct-injection (H2DDI)**

⇨ **NH_3-H_2 TJI engine**

2 × fuels = complex²

Efficiency/accuracy of tabulated kinetics

TCI essential

Kinetics to be continuously improved
⇨ Also for conventional fuels

H2DDI:

- PDF+FGM valid for diffusion mode
- EMCF+FGM more flexible, efforts needed to engine adaptation

NH_3-H_2 TJI:

- Laminar flame speed at $\phi > 1.5$
- SACI operation to be included

Ack.: A. Dupuy, R. Rabello de Castro, P. Brequigny, C. Mounaïm-Rousselle (Uni. Orléans)

THANK YOU

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