Tri-Fuel Combustion: Spray Assisted Ignition of Methanol-Hydrogen Blends

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Gadalla, Kaario et all, Int. Journal of Hydrogen Energy, 2021

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Outline

Background and motivation

-Dual-fuel (DF) and Tri-fuel (TF) ignition concept

Objectives and numerical setup

-0D and 3D ECN Spray A baseline

Results and conclusions

-0D and LES

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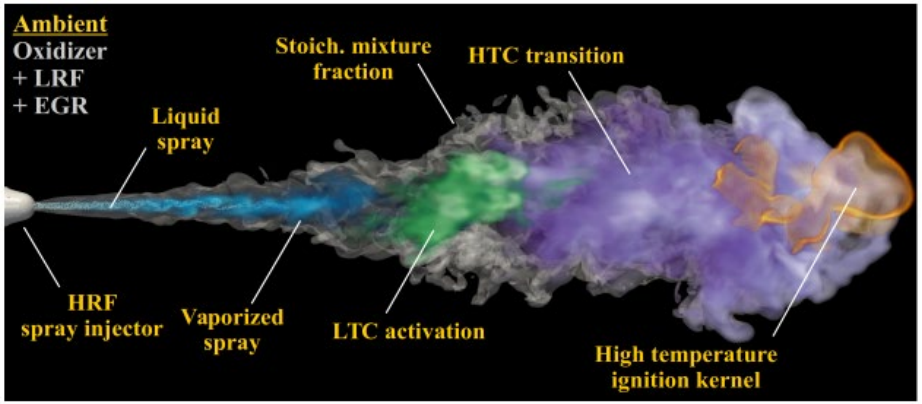
Dual-fuel and tri-fuel spray-assisted ignition concept

- Direct injection of the high-reactivity fuel (HRF)
- Lean **premixed** charge comprising of **low reactivity fuel** (LRF) and oxidizer/EGR.
- LRF is introduced to deliver the primary energy

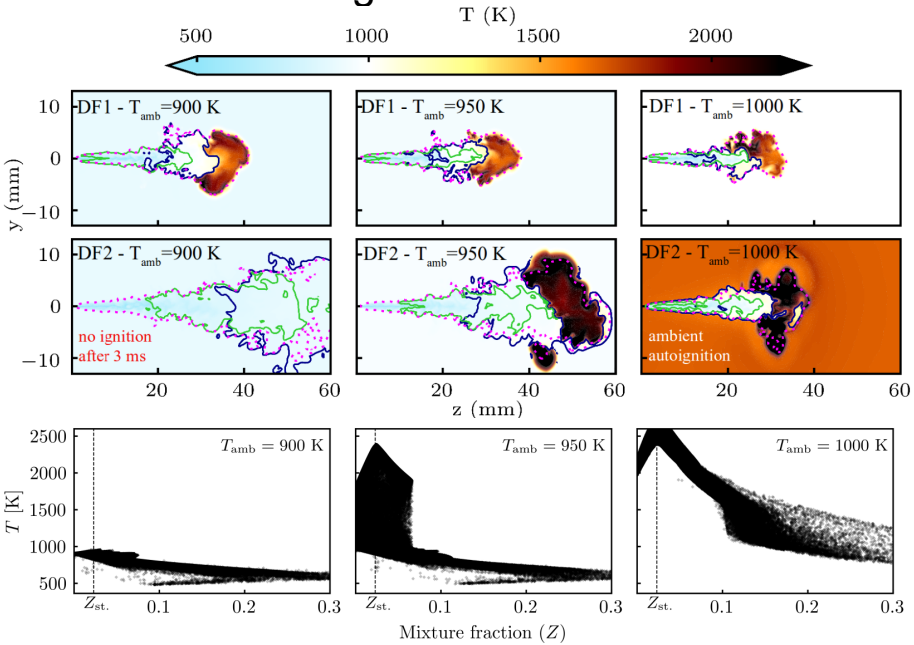
- DF/TF combustion:
  - Dependence on LRFs (methane/methanol/hydrogen) instead of diesel: renewable, low Carbon content (low PM).
  - Lean burn: allows to i) achieve low temperature combustion (minimize NOx), ii) minimize soot emissions.



TF H2 / Methanol - Motivation

- **Motivation** of this TF work (H2/CH3OH) originates from previous work on methanol versus methane DF at various ambient temperatures (Karimkashi et al., Int. Journal of Engine Research, 2022)
- HRF: n-dodecane. LRF: methane (DF1) or methanol (DF2)
- Tinj = 363 K, Pinj = 150 MPa, ρ_{amb} = 22.8 Kg/m3, O2= 15 %mol, **T_{amb} =varied**
- **Narrow T_{amb} operational window** for smooth ignition was observed for methanol (DF2)

Hypothesis: Adding H2 will have the potential to extend the narrow operational window for DF methanol.



Objectives and Numerical setup

Objectives:

- Use 0D modeling to explore the parameter space in terms of T_{amb}, ϕ_{amb}, and β = [H2]/([H2] + [CH3OH]) to extend the narrow operational window of methanol utilization
- Use 3D modeling to investigate effects of various blends of H2/methanol and the ignition characteristics in TF context.

Spray and ambient conditions (modified ECN Spray A):

- Computational volume is consistent with Sandia combustion vessel.
- Tinj = 363 K, Pinj = 150 MPa, T_{amb} = 900 K, ρ_{amb} = 22.8 Kg/m3, O2= 15 %mol.

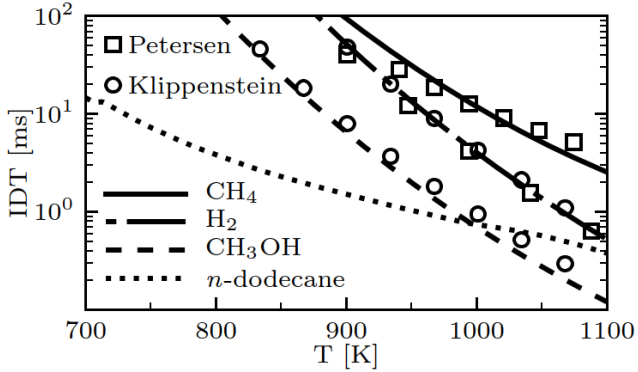
Framework: based on OpenFOAM with finite-rate chemistry. Reduced chemical mechanism (Frassoldati et al., CnF 2015). Chemistry solver is optimized via dynamic load balancing (DLB) and analytical Jacobian.

		SF	DF	TF-80	TF-85	TF-90	TF-95	TF-100
T_{amb}	[K]	900	900	900	900	900	900	900
T_{liq}	[K]	363	363	363	363	363	363	363
ρ	[Kg/m^3]	22.8	22.8	22.8	22.8	22.8	22.8	22.8
β_X		—	0.0	0.80	0.85	0.90	0.95	1.0
O_2	[%, mol]	15.0	15.0	15.0	15.0	15.0	15.0	15.0
N_2	[%, mol]	75.15	70.729	65.677	64.948	64.098	63.093	61.888
CO_2	[%, mol]	6.23	5.864	5.445	5.384	5.314	5.231	5.131
H_2O	[%, mol]	3.62	3.407	3.164	3.129	3.088	3.039	2.981
CH_3OH	[%, mol]	0.0	5.0	2.143	1.731	1.25	0.682	0.0
H_2	[%, mol]	0.0	0.0	8.571	9.808	11.25	12.955	15.0
ϕ_{amb}		0.0	0.5	0.5	0.5	0.5	0.5	0.5
$Z_{st.}$		0.0435	0.0229	0.0249	0.0252	0.0256	0.0261	0.0266

TF H2/methanol – 0D analysis

- **At 1000 K:** H2 ignition delay is much longer than methanol IDT

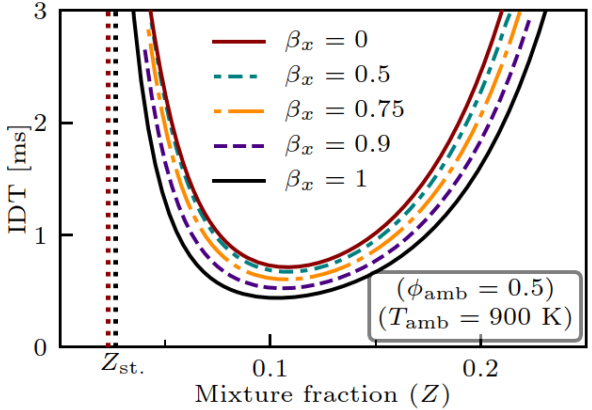
Single-fuel (SF) results



1000K: Add H2 to mitigate the ambient auto-ignition (without n-dodecane)

- **At 900 K**: H2 advances n-dodecane/methanol IDT

Dual-fuel (DF) / tri-fuel (TF) results



Therefore, **adding H2 extends the operational window for methanol DF ignition**

Shervin, Kaario, Vuorinen et all, Int. Journal of Hydrogen Energy, 2020

TF H2/methanol – 0D analysis

Combined effects of T_{amb}, ϕ_{amb}, and β variations on IDT_{MR}
Hatched regions denote autoignition at Z = 0 (no n-dodecane)

		SF	DF	TF-80	TF-85	TF-90	TF-95	TF-100
T_{amb}	[K]	900	900	900	900	900	900	900
T_{liq}	[K]	363	363	363	363	363	363	363
ρ	[Kg/m^3]	22.8	22.8	22.8	22.8	22.8	22.8	22.8
β_X		—	0.0	0.80	0.85	0.90	0.95	1.0
O_2	[%, mol]	15.0	15.0	15.0	15.0	15.0	15.0	15.0
N_2	[%, mol]	75.15	70.729	65.677	64.948	64.098	63.093	61.888
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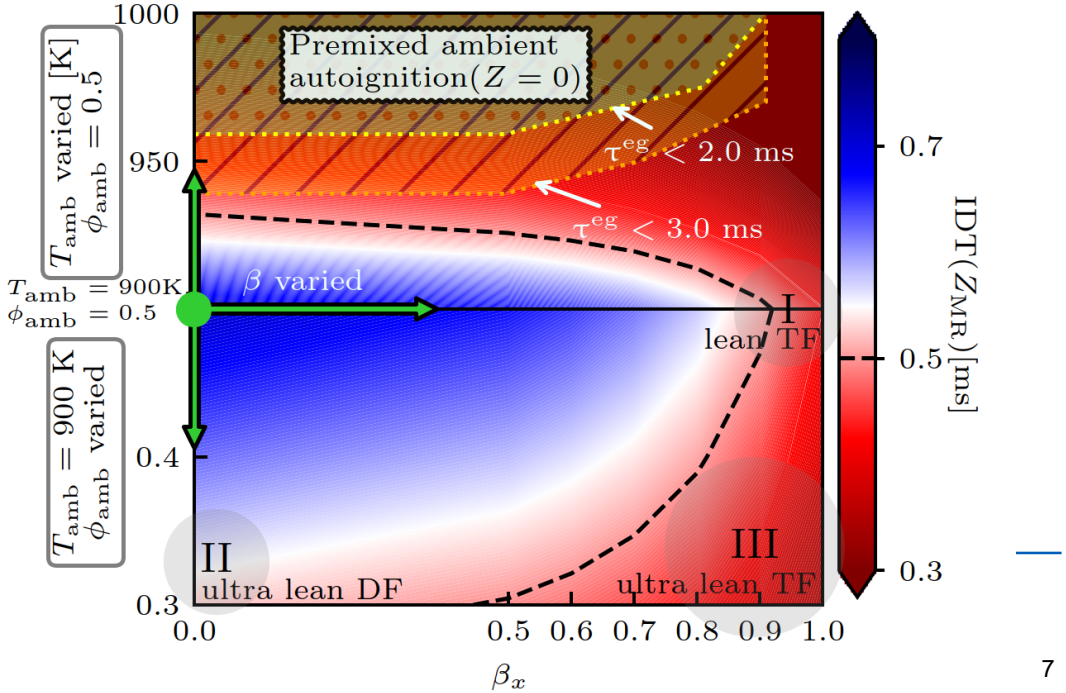
ϕ_{amb}		0.0	0.5	0.5	0.5	0.5	0.5	0.5
$Z_{st.}$		0.0435	0.0229	0.0249	0.0252	0.0256	0.0261	0.0266

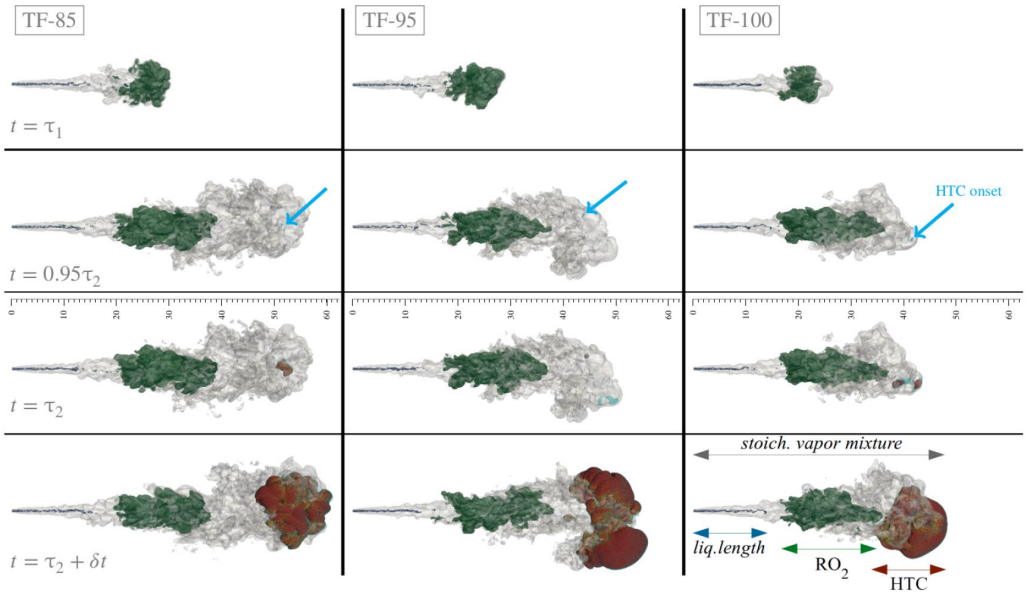
IDT can be advanced through
i) more H2
ii) lower ϕ_{amb}
iii) higher T_{amb}

Ambient autoignition is mitigated with more H2



TF H2/methanol – LES analysis

- Five testcases (TF-80 – TF-100) are prepared. Below are qualitative and quantitative results.
- **Adding H2 advances IDT also in 3D**



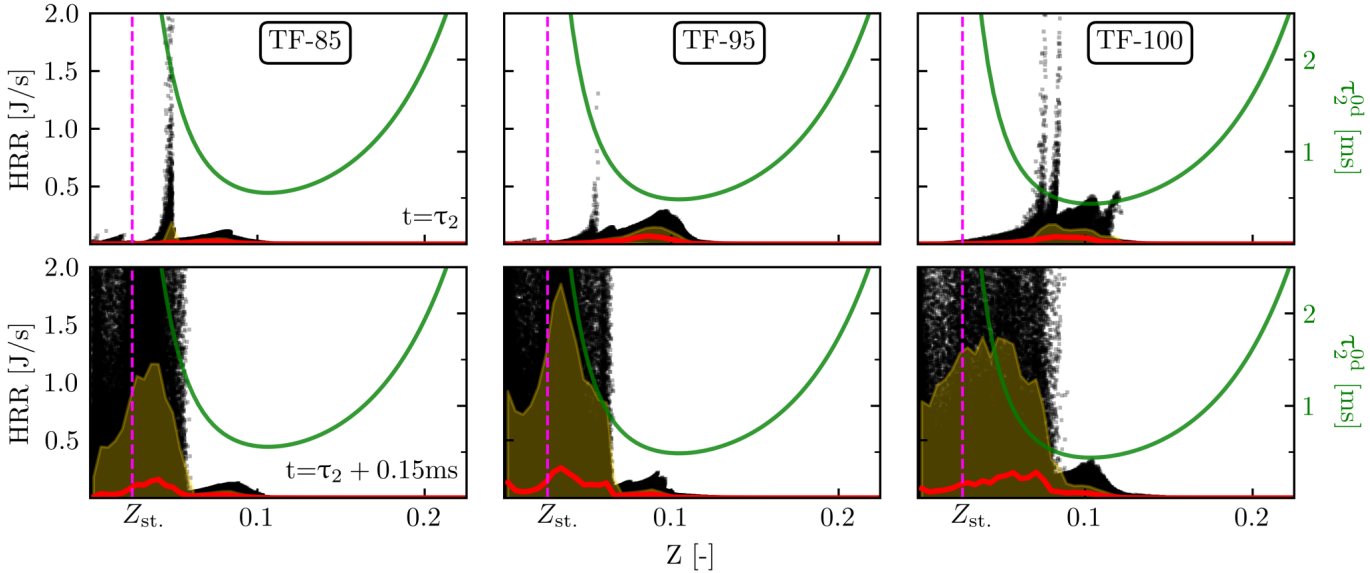
Gray color = stoichiometric surface
Green color = RO2
Red color = Temp > 1600k

	τ_1 [ms]	τ_2 [ms]	τ_2/τ_1	τ_2/IDT^{0d}_{MR}	L_{liq} [mm]	$L_{vap}(\tau_2)$ [mm]
TF-80	0.43	1.66	3.85	2.875	14.15 ± 2.11	62.00
TF-85	0.40	1.51	3.78	2.753	14.08 ± 2.04	56.73
TF-90	0.37	1.55	4.19	2.997	14.03 ± 2.09	55.90
TF-95	0.36	1.16	3.22	2.430	13.90 ± 2.30	50.87
TF-100	0.286	0.86	3.01	2.003	13.80 ± 2.38	43.71

TF H2/methanol – LES analysis

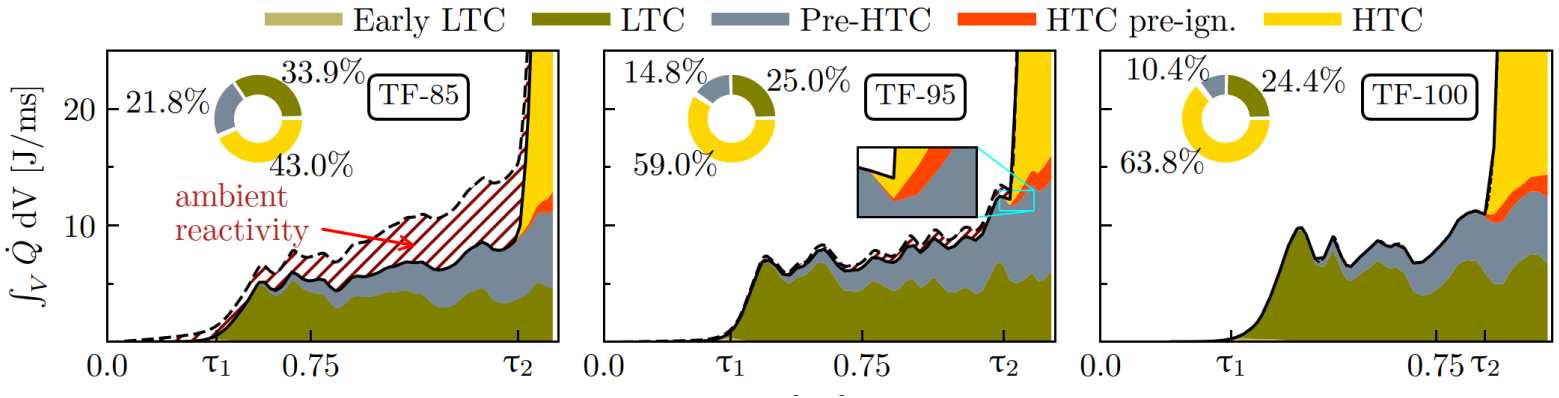
- Heat release analysis: **scatter plots** from 3D data
- HRR peaks (i.e. first ignition kernels) occur on rich Z, (spray-assisted concept).
- With more H2:
  - Most reactive mixture is richer in Z space (i.e. shorter spray and IDT).
  - Most reactive mixture converges to that in 0D (less mixing time).
  - Later, larger equivalence ratio range

Red line = Cond HRR
Green area = std dev.



TF H2/methanol – LES analysis

Heat release maps – Ignition mode decomposition (T=900K)



- Hatched zone denotes ambient reactivity. Pie chart is cumulative HRR mode.
- **With more H2:**
  - Ambient heat release is mitigated
  - HTC share to THRR is larger

Table 4: Criteria for ignition modes. $RO2^\star=10^{-5}$, $H2O2^\star=10^{-4}$, $OH^\star=10^{-5}$, $T^\star=1150$ K

Mode	Definition
Early LTC	$(RO2 \geq 10^{-7}) \cap (H2O2 < H2O2^\star) \cap (T < T^\star)$
LTC	$(RO2 \geq RO2^\star) \cap (H2O2 \geq H2O2^\star) \cap (T < T^\star)$
Pre-HTC	$(RO2 < RO2^\star) \cap (H2O2 \geq H2O2^\star) \cap (T < T^\star)$
HTC pre-ign.	$(OH < OH^\star) \cap (T \geq T^\star)$
HTC	$(OH \geq OH^\star) \cap (T \geq T^\star)$

TF H2/methanol - Summary

1. The multi-parametric 0D analysis suggests that a narrow smooth ignitability window of methanol DF can be extended via H2 enrichment. **Advantage of adding H2 is two-fold:** i) its lower reactivity compared with methanol potentially avoids the ambient autoignition without HRF, and ii) its reactivity-promoting effects could advance IDT.

2. **First and second stage IDT are advanced with H2**. Moreover, having twice H2 blending mass ratio (25%-50% or 50%-100%) in the premixed charge is advancing IDT by 23-26%, with shorter penetrations (10-15%) of the vaporized spray.

3. According to ignition mode decomposition analysis, ambient reactivity persists in the system which might raise concerns regarding abnormal ignition or cyclic instability. More than 50% of H2 mass ratio (94% molar) is required to ensure a non-reactive ambient.

Gadalla, Kaario, Vuorinen et all, Int. Journal of Hydrogen Energy, 2021