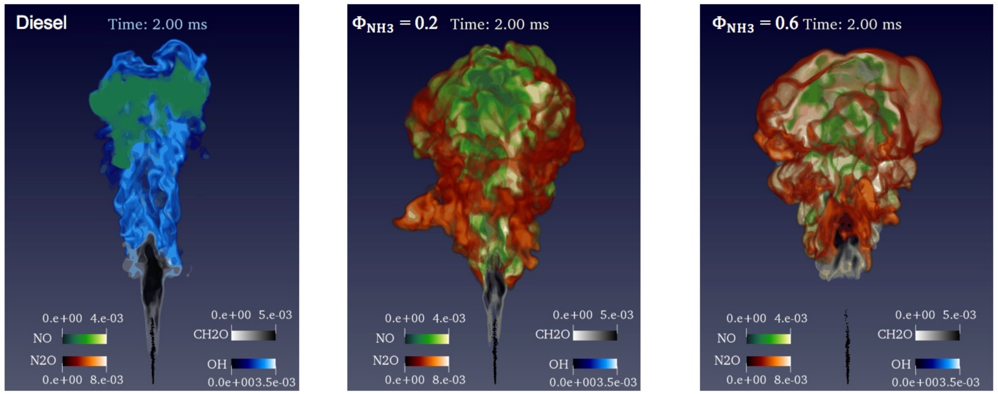
Concepts of Ammonia/Hydrogen Engines for Marine Application – CFD modeling

Nordic Maritime Transport and Energy Research Programme Workshop, April 20-21, 2022



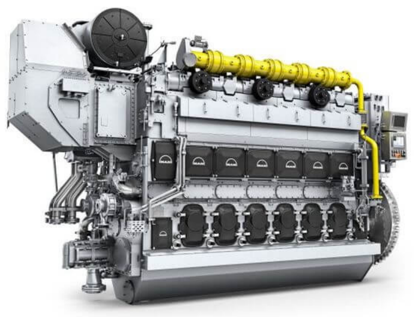
Xue-Song Bai, Leilei Xu, Mark Treacy, Lund University

www.fm.energy.lth.se

Outline

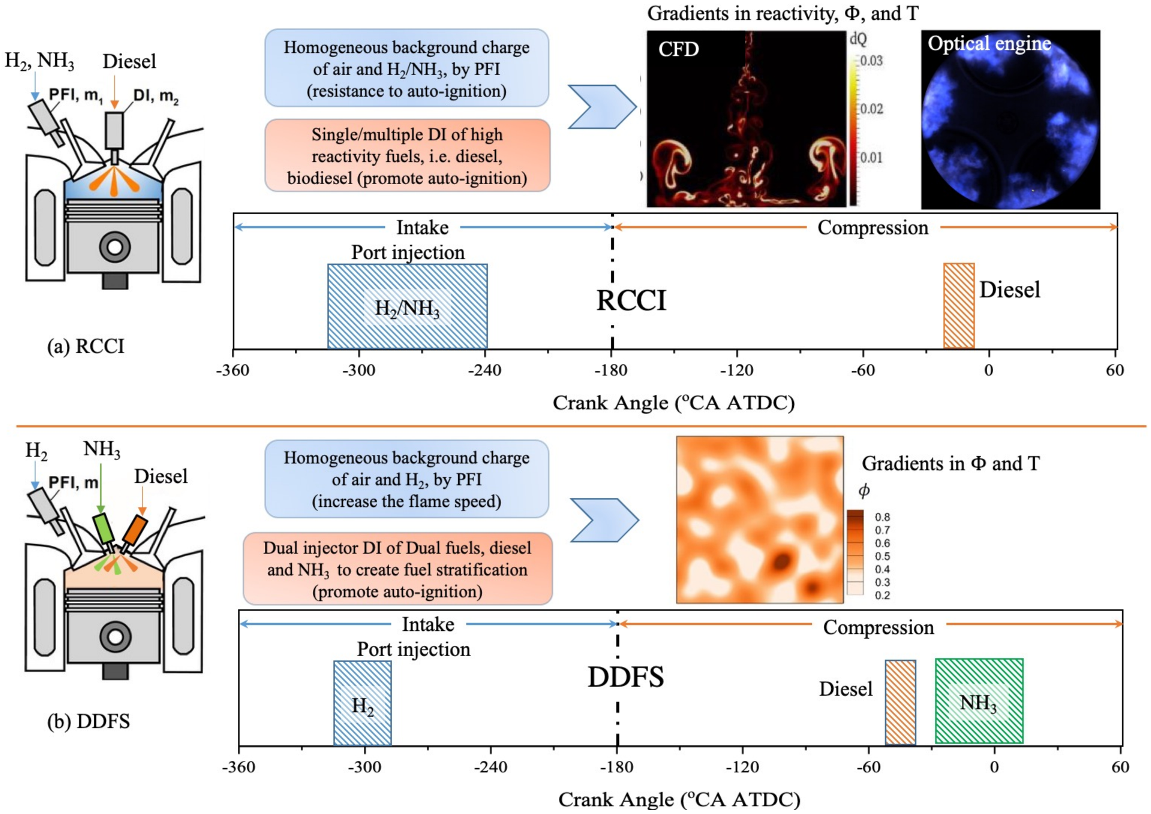
- CAHEMA - Concepts of Ammonia/Hydrogen Engines for Marine Application
- CFD study of ammonia/hydrogen/n-heptane RCCI engine performance
  - LES study of n-heptane/ammonia RCCI ignition
  - RANS study of a four-stroke n-heptane/ammonia/hydrogen RCCI engine
- Concluding remarks and future work

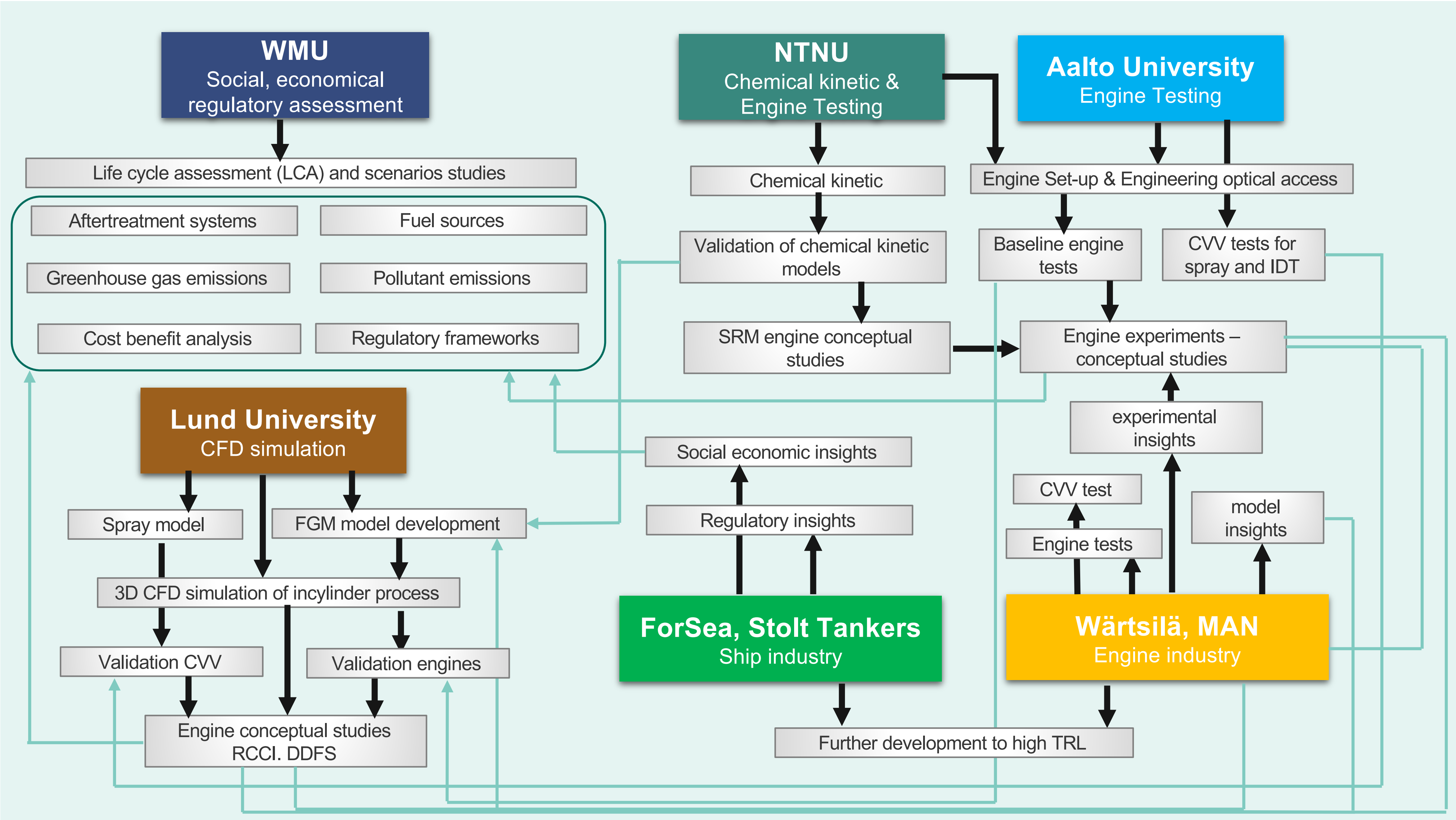
Concepts of Ammonia/Hydrogen Engines for Marine Application



MAN ES AMMONIA ENGINE PROJECT - AENGINE

WÄRTSILÄ AMMONIA AND HYDROGEN RESEARCH





WMU
Social, economical regulatory assessment
Life cycle assessment (LCA) and scenarios studies
Aftertreatment systems
Fuel sources
Greenhouse gas emissions
Pollutant emissions
Cost benefit analysis
Regulatory frameworks
NTNU
Chemical kinetic & Engine Testing
Chemical kinetic
Validation of chemical kinetic models
SRM engine conceptual studies
Aalto University
Engine Testing
Engine Set-up & Engineering optical access
Baseline engine tests
CVV tests for spray and IDT
Engine experiments – conceptual studies
experimental insights
CVV test
Engine tests
model insights
Lund University
CFD simulation
Spray model
FGM model development
3D CFD simulation of incylinder process
Validation CVV
Validation engines
Engine conceptual studies RCCI. DDFS
Social economic insights
Regulatory insights
ForSea, Stolt Tankers
Ship industry
Wärtsilä, MAN
Engine industry
Further development to high TRL

LES of n-heptane spray in ammonia/air mixture under RCCI conditions

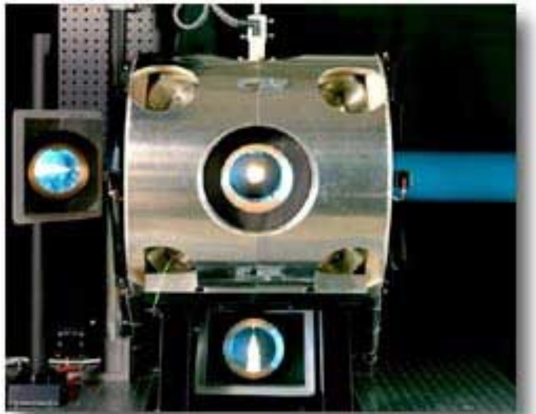
Case Setup

ECN (engine Combustion Network) – test rig
https://ecn.sandia.gov/diesel-spray-combustion/sandia-cv/

CAHEMA

ECN Spray H	
Diameter (mm)	0.1
Injected fuel	N-heptane
Duration (ms)	6
Injection pressure (MPa)	150

Ambient conditions （based on Spray H）	
Temperature (K)	900
Pressure (MPa)	3.81
Density (kg/m^3)	15.0
Φ_a (ambient premixed NH3/air)	0, 0.2, 0.4, 0.6



Sandia CV

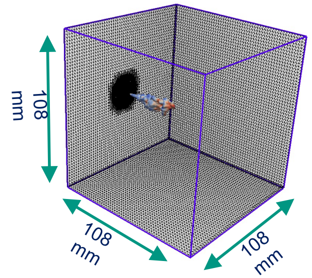
- Ambient gas temperatures from 450 K to 1300 K
- Ambient gas densities from 3 to 60 kg/m^3
- Ambient gas oxygen concentrations from 0% to 21%

- Injection pressures above ambient from 40 to 200 MPa
- Nozzle sizes from 0.05 to 0.5 mm
- #2 diesel, single-component reference (n-heptane, cetane), and oxygenated fuels

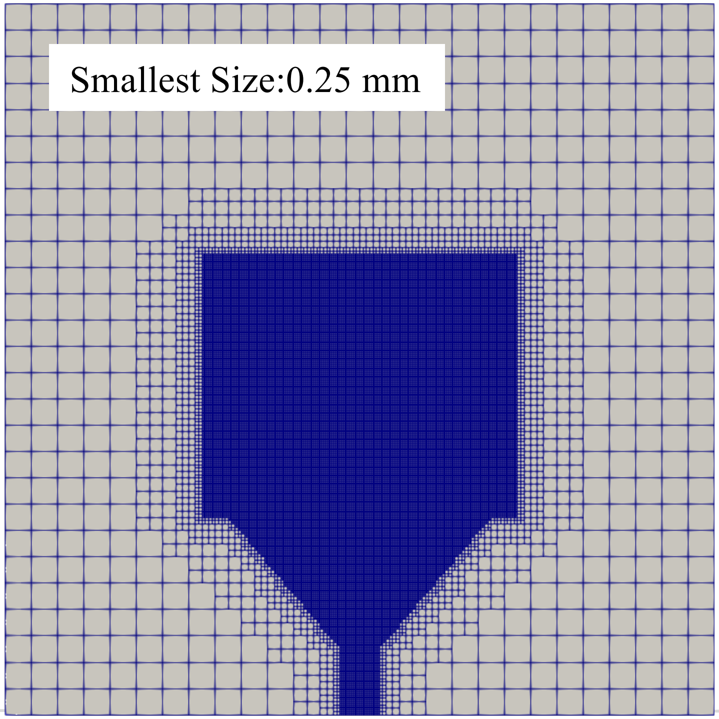
Case Setup

ECN Spray H	
Diameter (mm)	0.1
Injected fuel	N-heptane
Duration (ms)	6
Injection pressure (MPa)	150

Ambient conditions （based on Spray H）	
Temperature (K)	900
Pressure (MPa)	3.81
Density (kg/m^3)	15.0
Φ_a (ambient premixed NH3/air)	0, 0.2, 0.4, 0.6

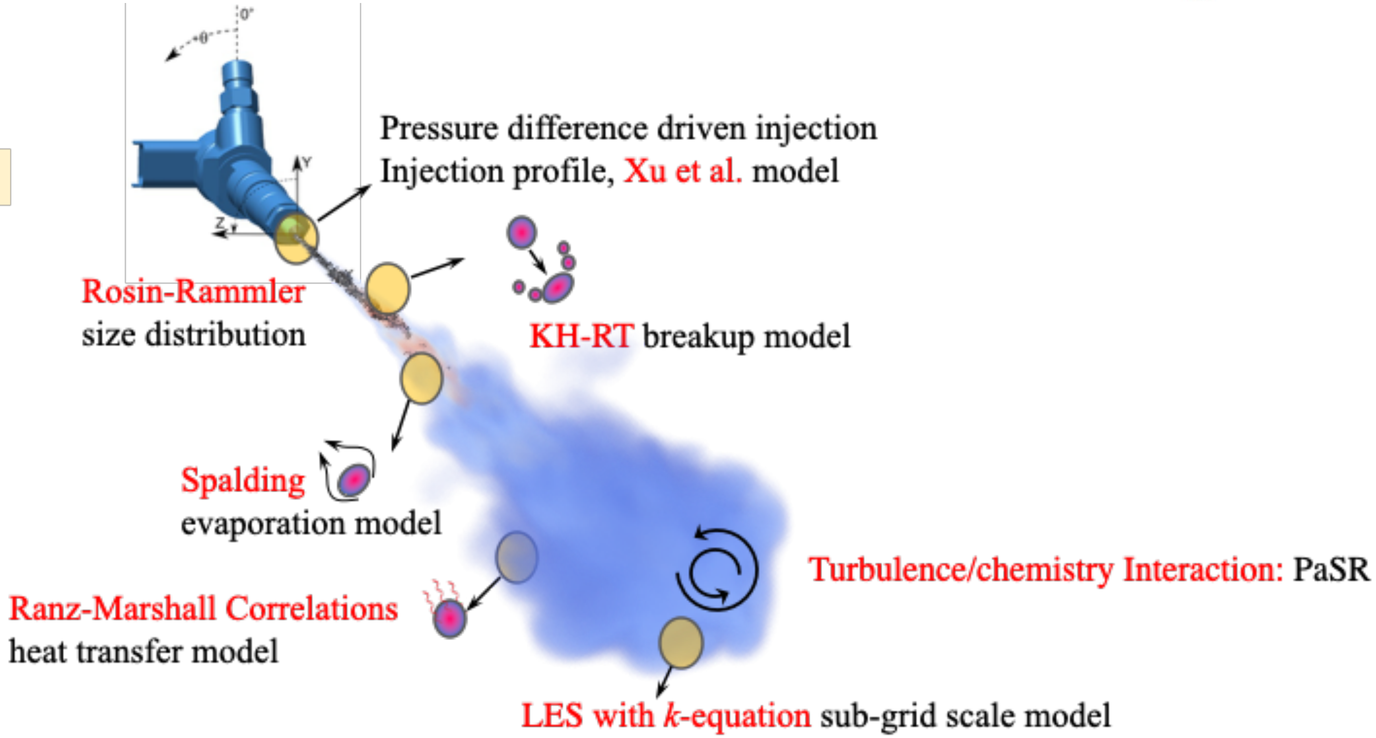


Charging homogeneous and quiescent ammonia-air mixture



LES model and chemical kinetics

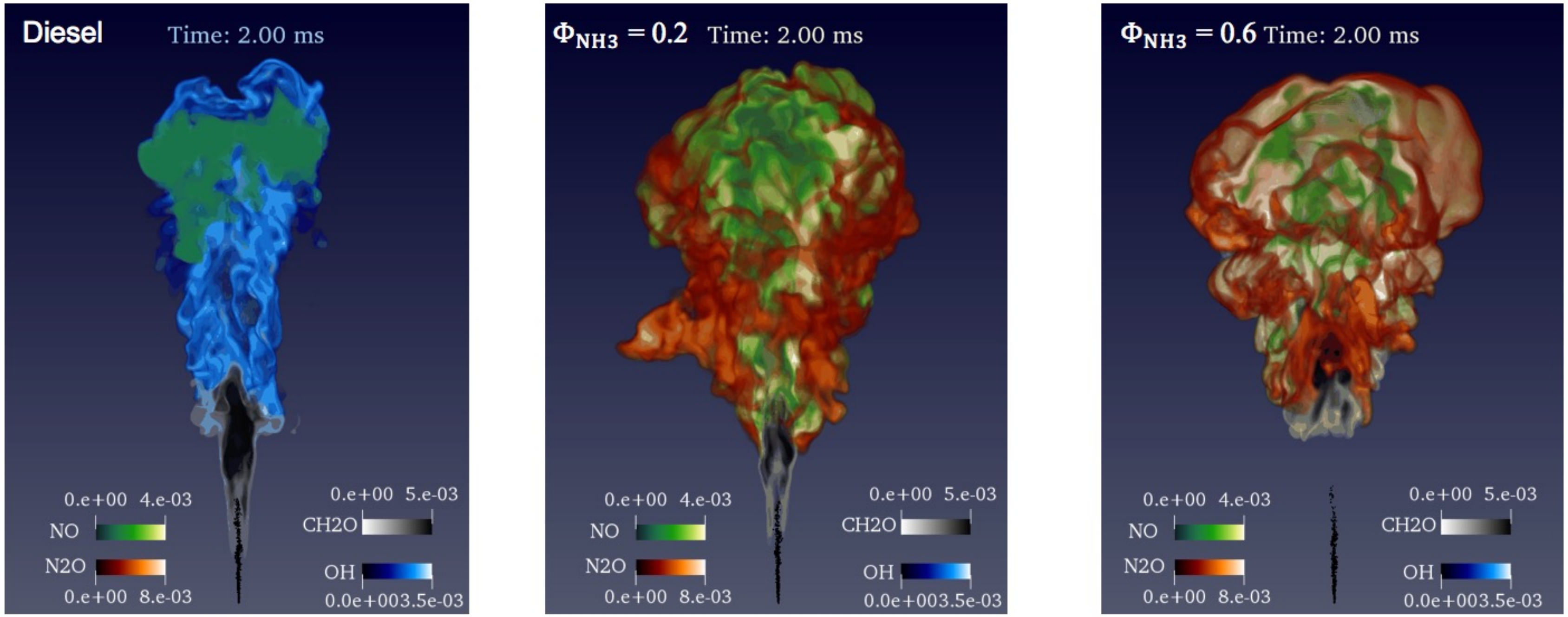
LPT approach



- Combustion mechanism: 69 species = 69 and 389 reactions.

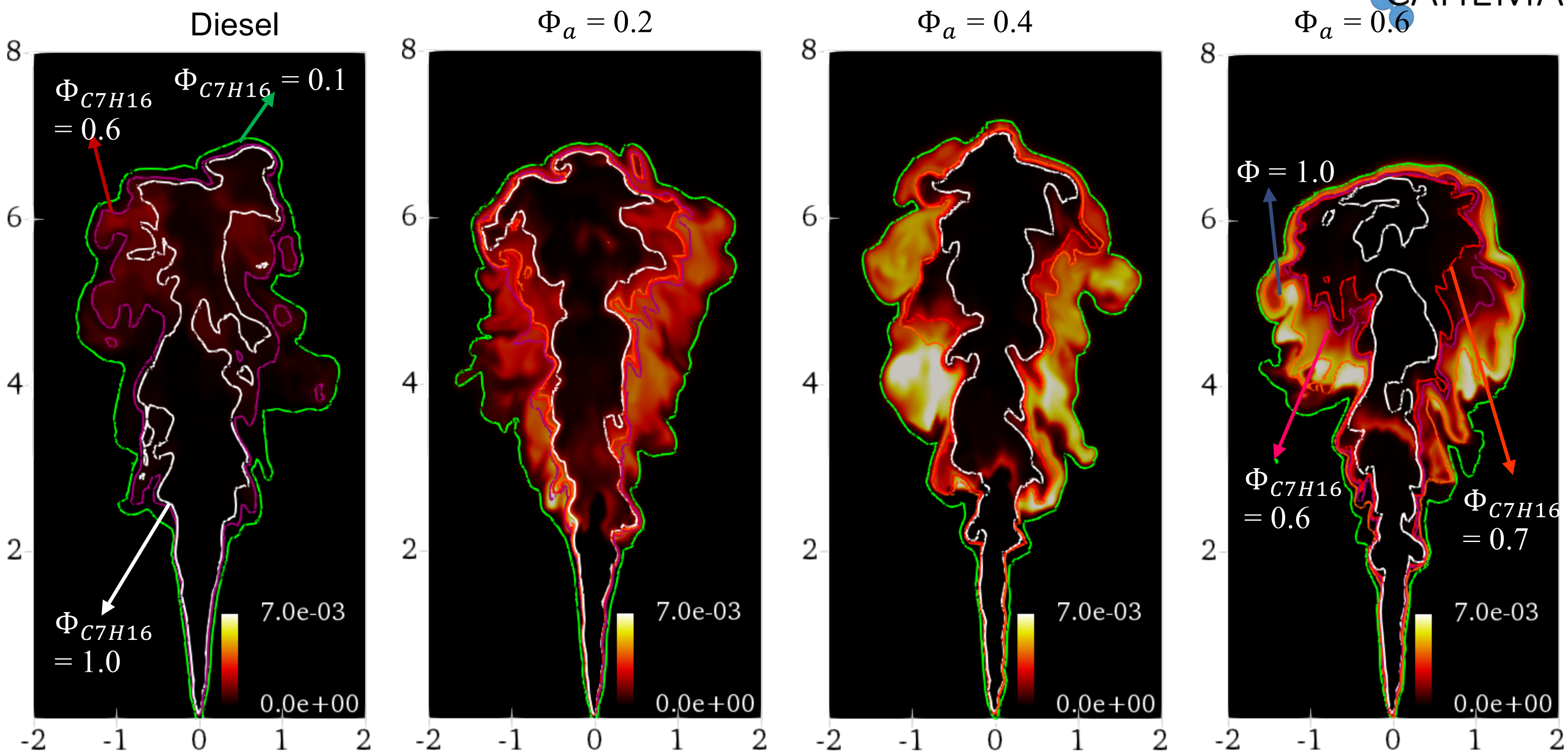
NH3/n-heptane combustion under RCCI conditions

- CH_2O: low temperature ignition
- OH: high temperature ignition
- NH_3 suppresses n-C7H18 auto-ignition



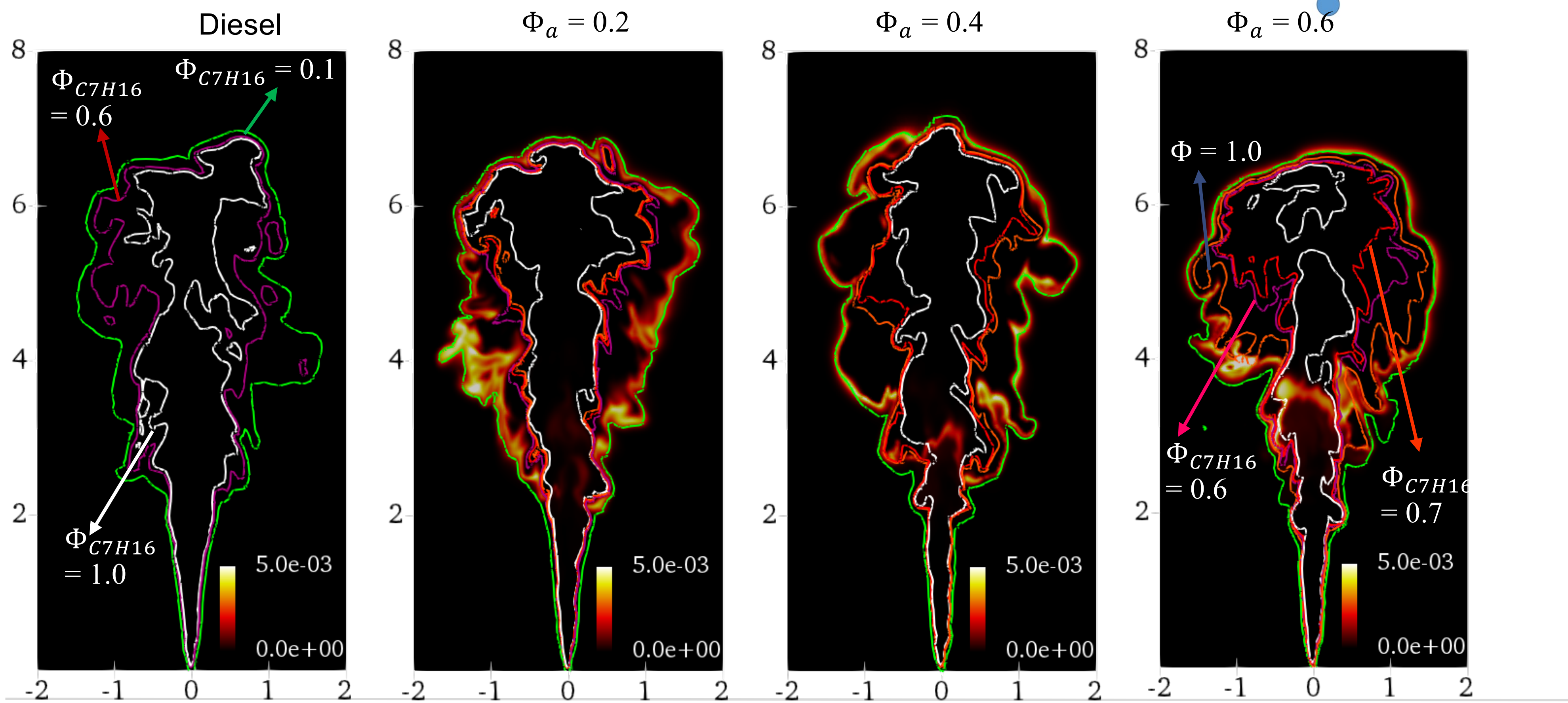
- Thermal NO: downstream high T
- N_2O is formed prior to NO formation
- NH_3 increases the liftoff length

NO



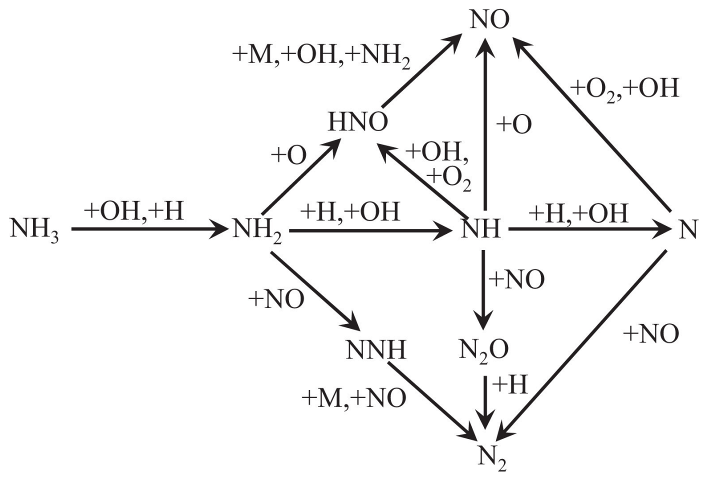
Diesel
$\Phi_a = 0.2$
$\Phi_a = 0.4$
$\Phi_a = 0.6$
$\Phi_{C7H16} = 0.6$
$\Phi_{C7H16} = 0.1$
$\Phi_{C7H16} = 1.0$
$\Phi = 1.0$
$\Phi_{C7H16} = 0.6$
$\Phi_{C7H16} = 0.7$
7.0e-03
0.0e+00
8
6
4
2
-2
-1
0
1
2

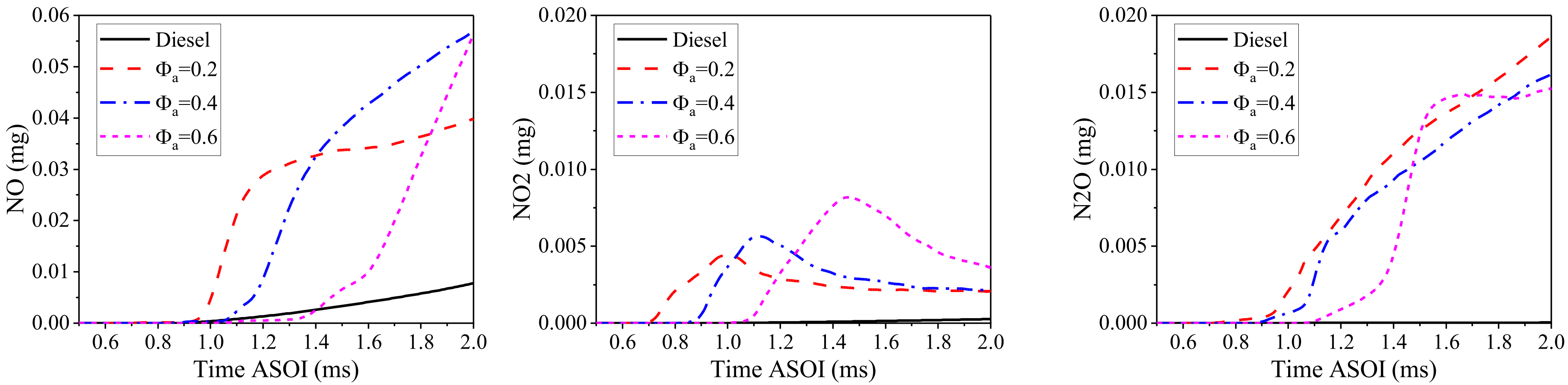
N2O



Diesel
$\Phi_a = 0.2$
$\Phi_a = 0.4$
$\Phi_a = 0.6$
$\Phi_{C7H16} = 0.6$
$\Phi_{C7H16} = 0.1$
$\Phi_{C7H16} = 1.0$
$\Phi = 1.0$
$\Phi_{C7H16} = 0.6$
$\Phi_{C7H16} = 0.7$
5.0e-03
0.0e+00
8
6
4
2
-2
-1
0
1
2

NO_x (NO, NO_2) and N_2O Emissions





LES results – major findings

- Ammonia suppresses the auto-ignition of diesel/n-heptane
  - The higher the ammonia/diesel ratio, the slower the diesel ignition
  - Implication to engine operation: earlier diesel injection
- NOx in the mixing layer
  - Thermal NO is formed in the downstream region of the flame
  - Fuel NO is several times of thermal NO
- N_2O formation and consumption
  - N_2O is formed prior to NO formation
  - N_2O is consumed when forming NO

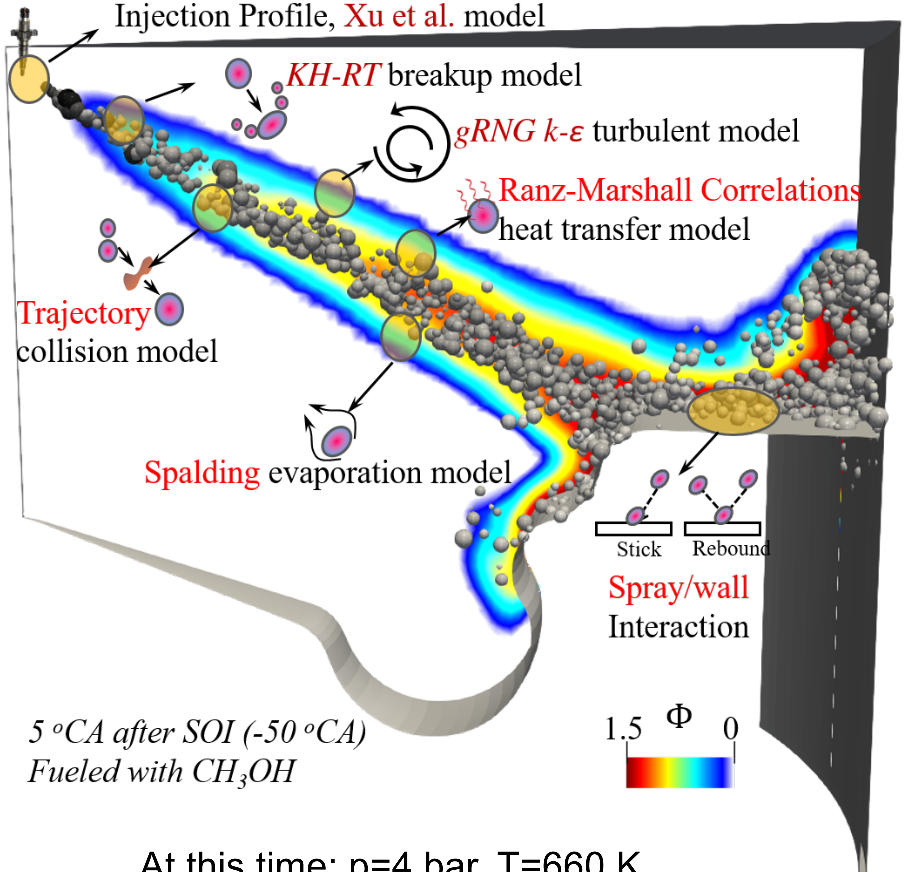
CAHEMA

RANS study of ammonia/hydrogen/n-heptane RCCI engine

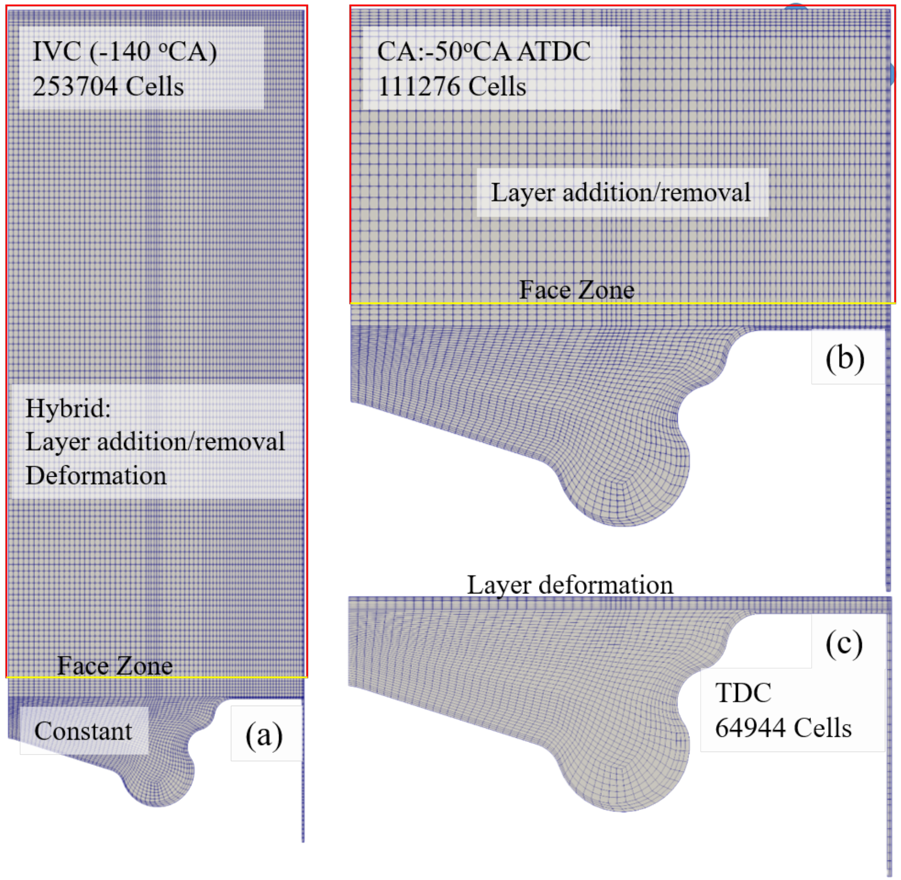
NER Workshop, 2022-04-20

Dept of Energy Sciences, Lund University

Numerical model



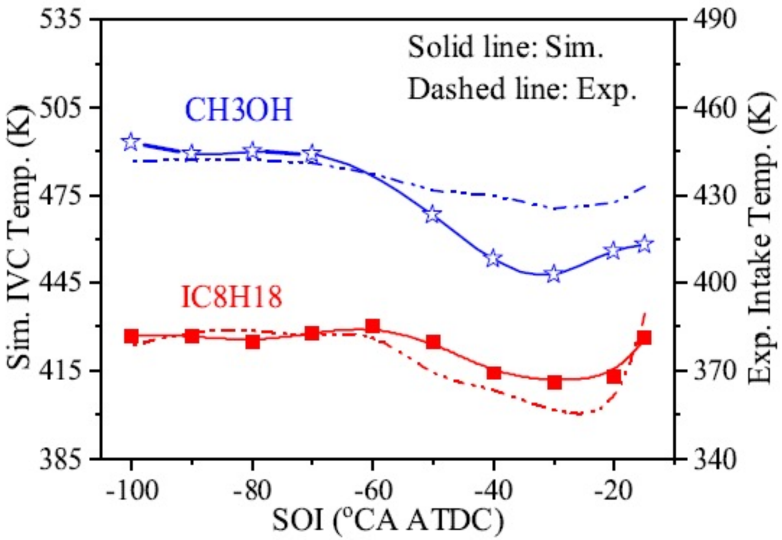
At this time: p=4 bar, T=660 K



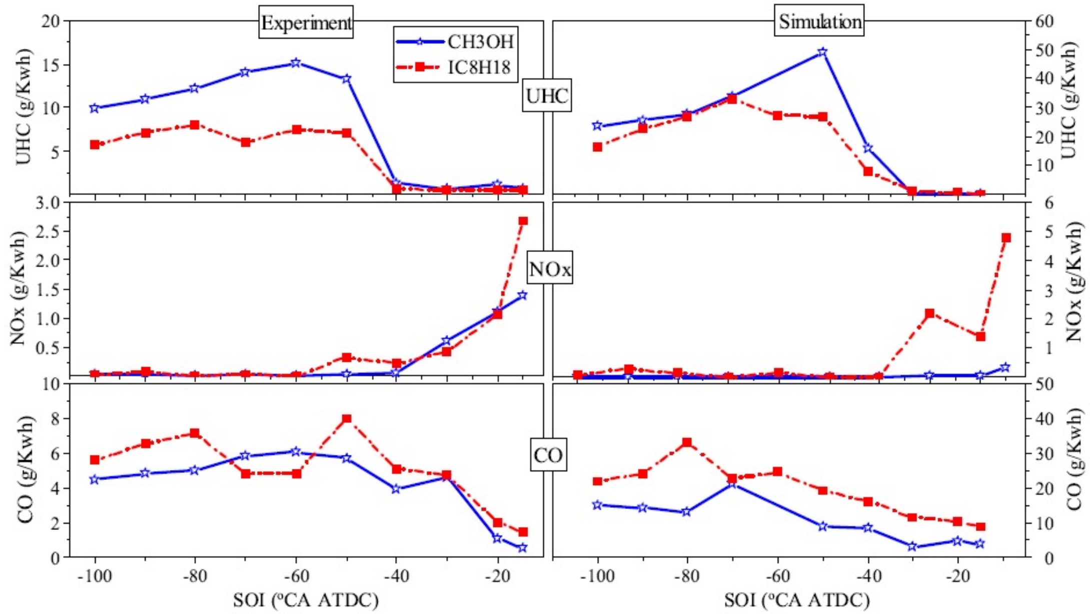
OpenFoam, sector mesh, 30 degree, 12 holes

Model Validation (methanol and iso-octane)

- Required **intake temperature** for marinating CA50 at 3 ^{o}CA ATDC for different SOIs



- **Emissions** at the different SOIs for both fuels



NH3 engine Case setup

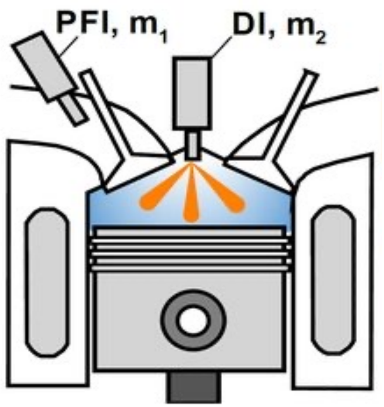
- RCCI concept, constant total energy (2kJ/cyc, engine load 4bar IMEP, similar to exp.);
- NH_3/H_2 is premixed with the air;
- IVC pressure：1.16651 bar, IVC Temperature：458 K;
- n-heptane (diesel) is injected at -7ᵒCA ATDC (Injection delay time 3ᵒCA @1200rpm)

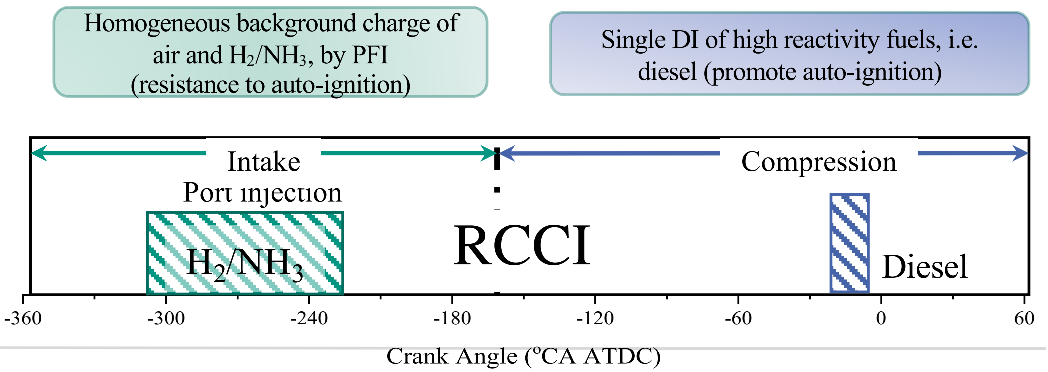
EP (**E**nergy **P**remixed):

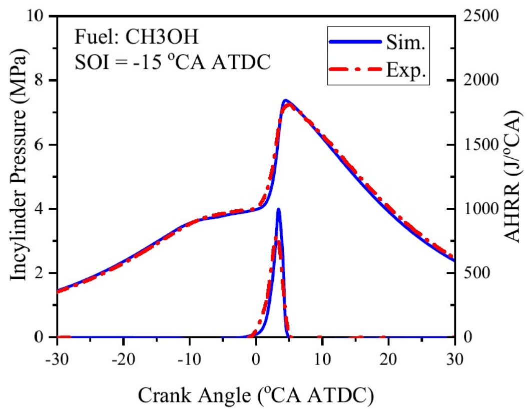
$$EP = \frac{m_{NH3} * LHV_{NH3} + m_{H2} * LHV_{H2}}{\text{Total Energy}}$$

X_{NH3} (**NH3 mole fraction**):

$$X_{NH3} = \frac{C_{NH3}}{C_{NH3} + C_{H2}}$$



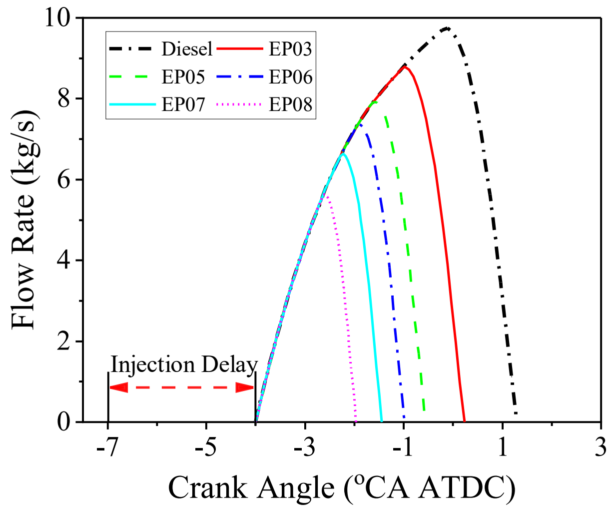


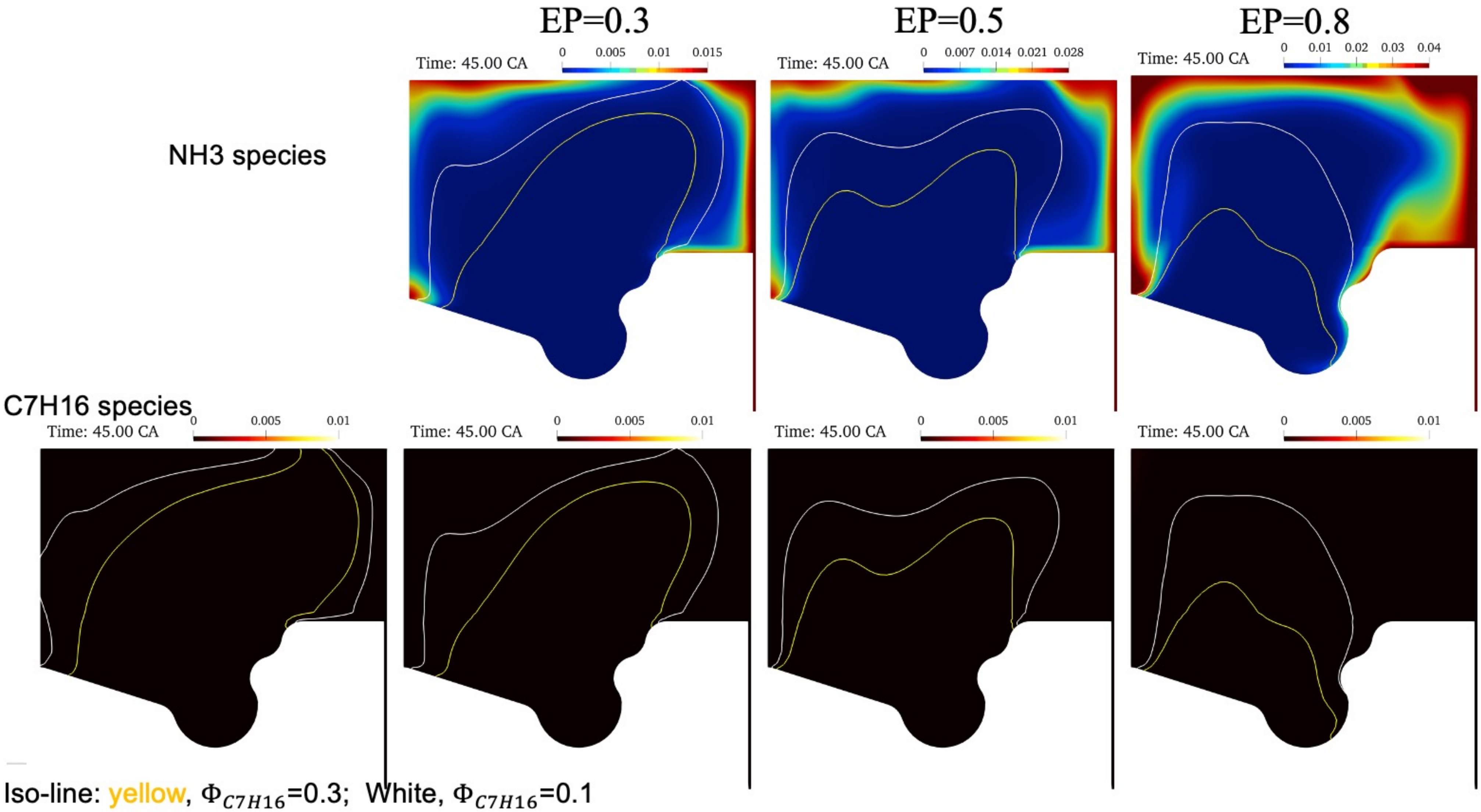


NH3 (premixed) + N-heptane (injected)

Total energy in the cylinder: 2000 J/cyc, 4 bar IMEP

Case Name	EP	X_{NH3}	Φ_0 (premix)	Injected Duration °CA (N-heptane)	Description
Diesel	0	0	0	5.292	Diesel Engine
EP03	0.3	1	0.106	4.230	RCCI engine
EP05	0.5		0.177	3.438	
EP06	0.6		0.212	3.015	
EP07	0.7		0.248	2.556	
EP08	0.8		0.283	2.034	

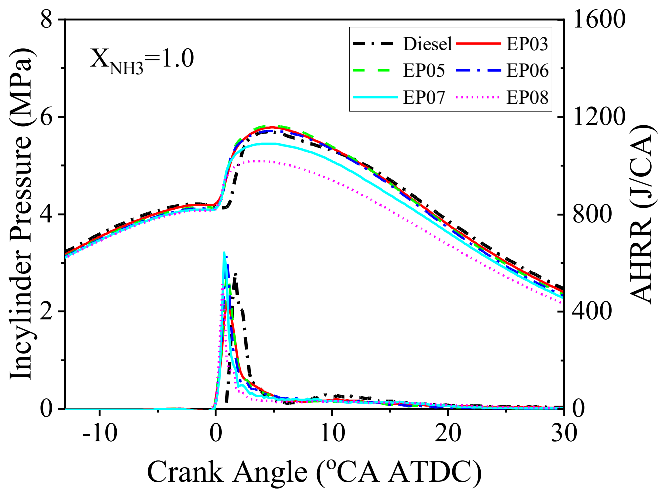


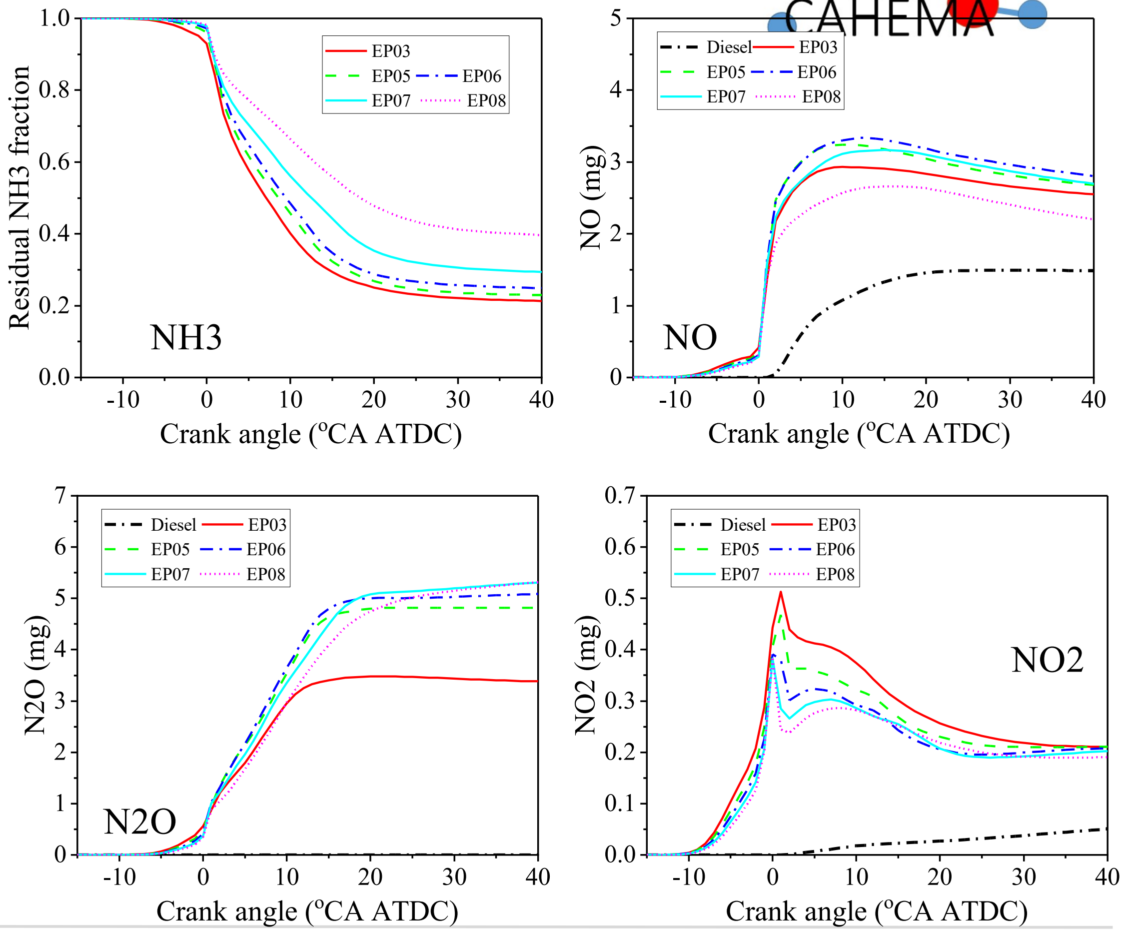


EP=0.3
EP=0.5
EP=0.8
NH3 species
C7H16 species
Time: 45.00 CA
0 0.005 0.01 0.015
0 0.007 0.014 0.021 0.028
0 0.01 0.02 0.03 0.04
0 0.005 0.01
Iso-line: yellow, Φ_{C7H16}=0.3; White, Φ_{C7H16}=0.1

NH3 Engine performance

- The ignition delay time for the NH3 RCCI engine is shorter due to the shorter injection;
- Ammonia is hardly burned completely;
- If the EP is greater than 0.5, the combustion efficiency of the ammonia becomes worse;
- N_2O/NO_2/NO emissions are much higher than that of diesel engine.



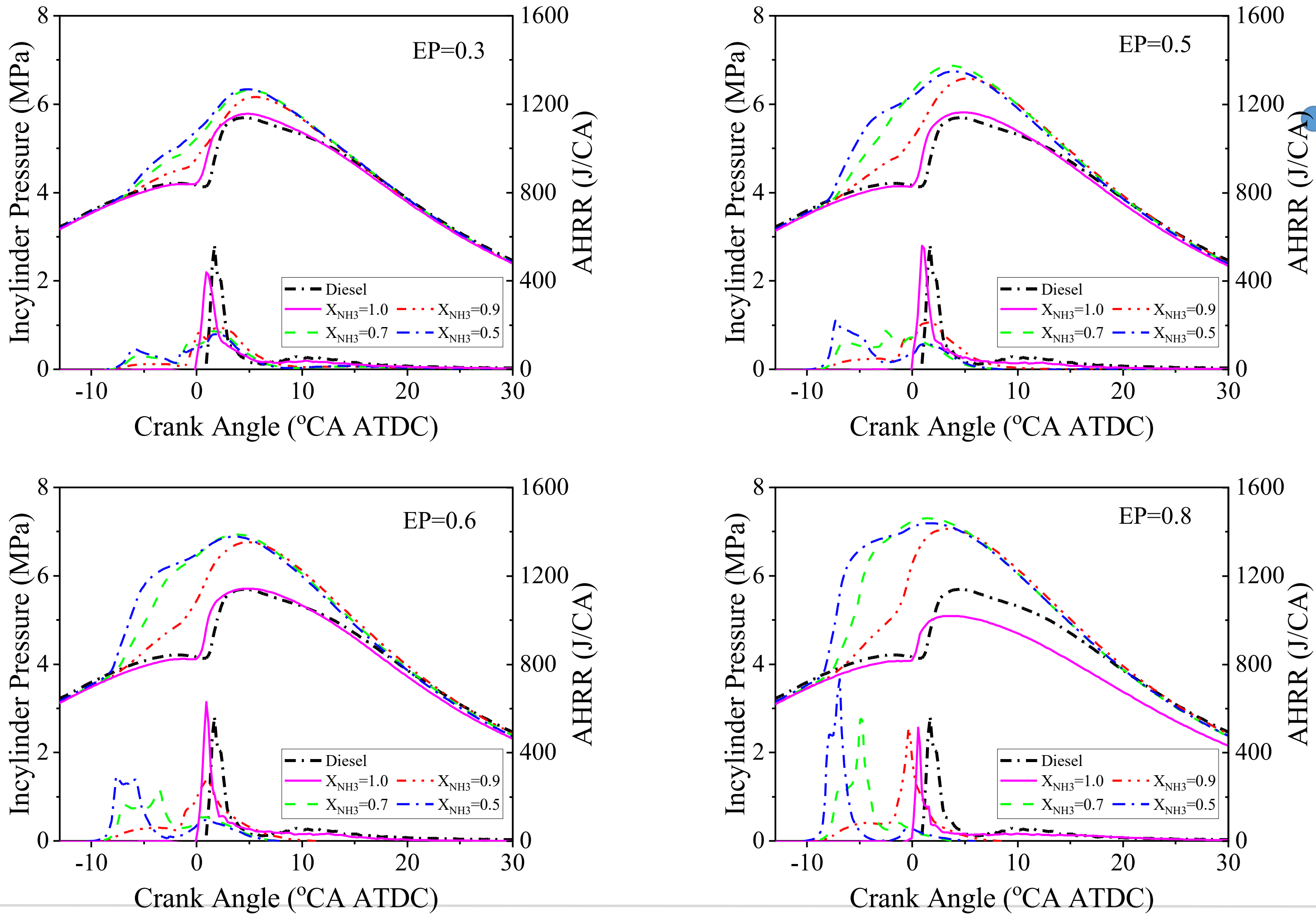


NH3/H2 (premixed) + N-heptane (injected)

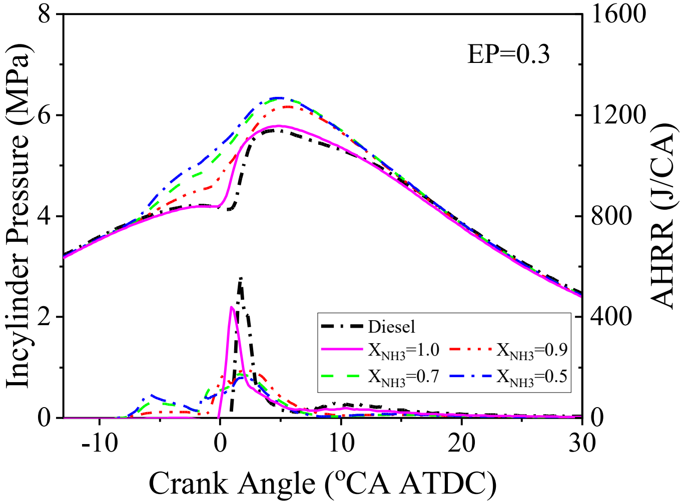
X_{NH3} (**NH3 mole fraction**):

$$X_{NH3} = \frac{C_{NH3}}{C_{NH3} + C_{H2}}$$

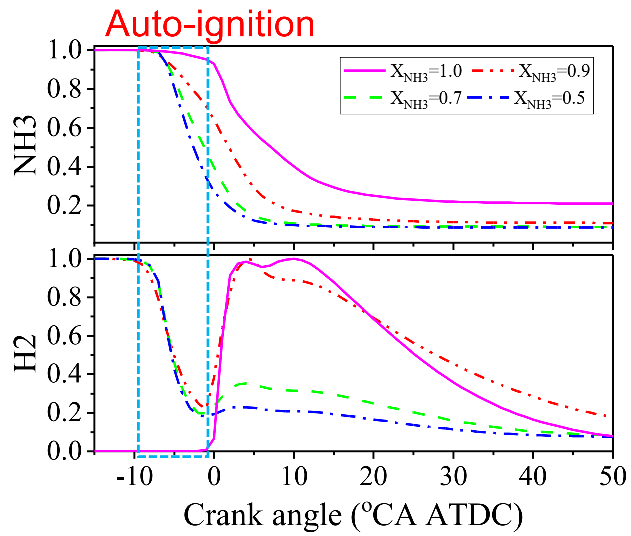
Case Name.	EP	Injected Duration °CA (N-heptane)	X_{NH3}	Φ_0 (premix)	X_{NH3}	Φ_0 (premix)	X_{NH3}	Φ_0 (premix)
EP03	0.3	4.230		**0.105**		**0.103**		**0.101**
EP05	0.5	3.438		**0.175**		**0.172**		**0.168**
EP06	0.6	3.015	**0.9**	**0.210**	**0.7**	**0.206**	**0.5**	**0.201**
EP07	0.7	2.556		**0.245**		**0.240**		**0.235**
EP08	0.8	2.034		**0.280**		**0.275**		**0.268**


EP=0.3
EP=0.5
EP=0.6
EP=0.8
Incylinder Pressure (MPa)
AHRR (J/CA)
Crank Angle (°CA ATDC)
Diesel
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5
0
2
4
6
8
0
400
800
1200
1600
-10
0
10
20
30

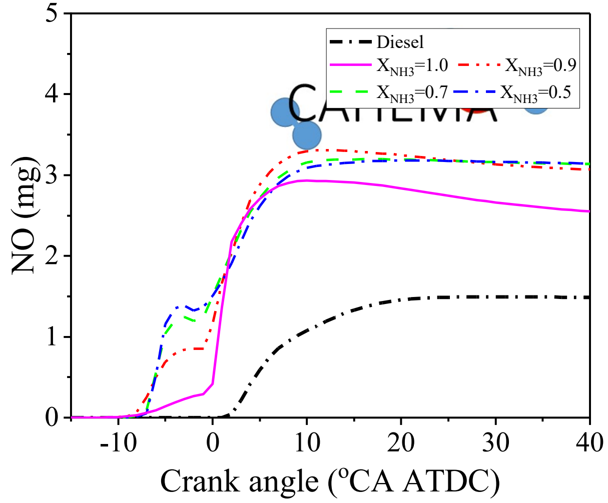
EP=0.3



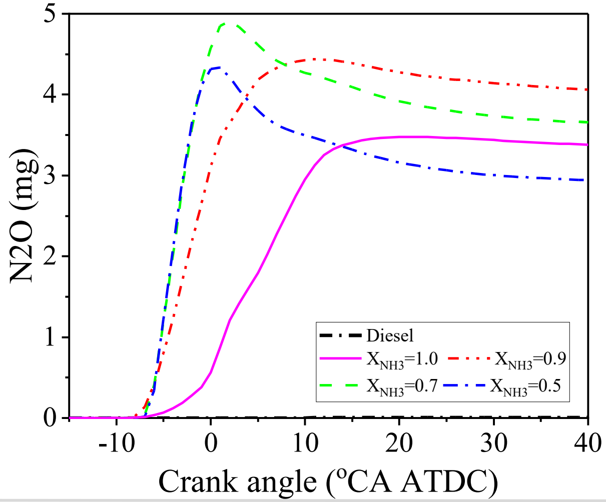
EP=0.3
Incylinder Pressure (MPa)
AHRR (J/CA)
Crank Angle (°CA ATDC)
Diesel
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5



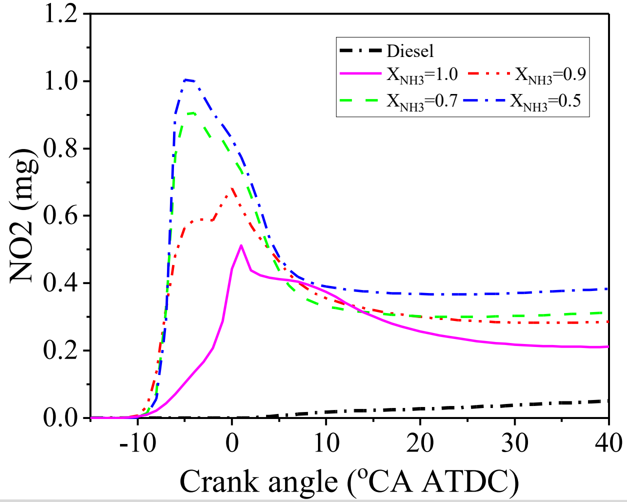
Auto-ignition
NH3
H2
Crank angle (°CA ATDC)
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5



NO (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5

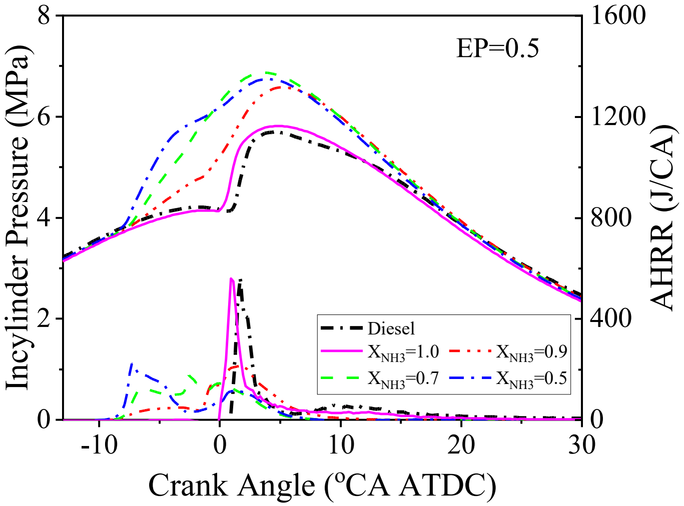


N2O (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5

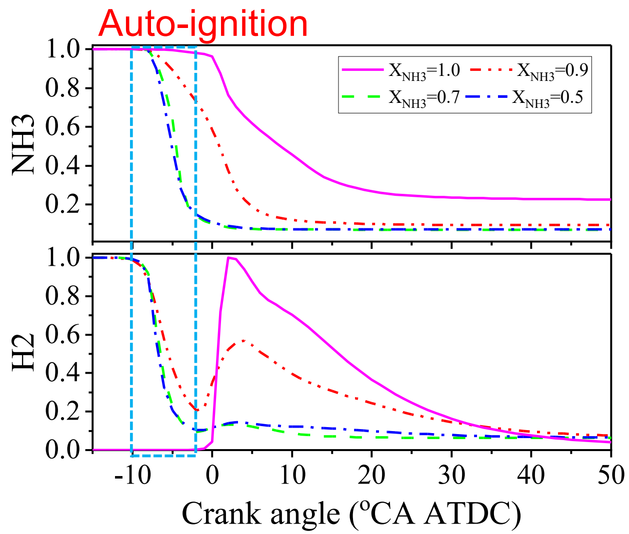


NO2 (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0
X_{NH3}=0.9
X_{NH3}=0.7
X_{NH3}=0.5

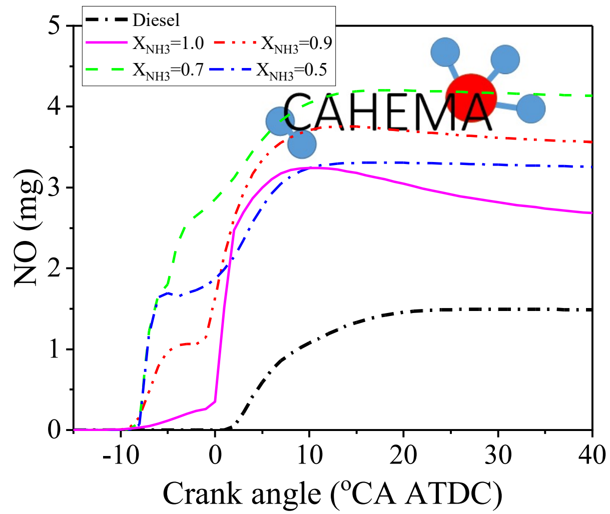
EP=0.5



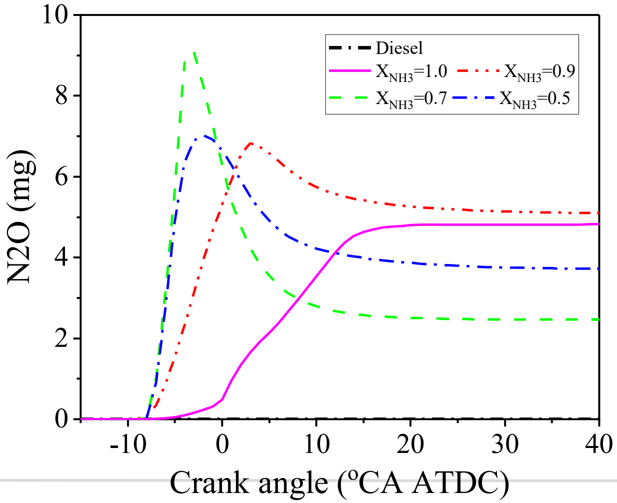
EP=0.5
Incylinder Pressure (MPa)
AHRR (J/CA)
Crank Angle (°CA ATDC)
Diesel
X_{NH3}=1.0 X_{NH3}=0.9
X_{NH3}=0.7 X_{NH3}=0.5



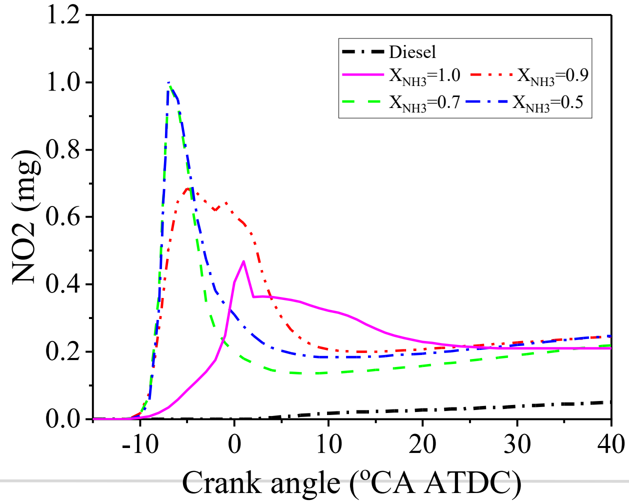
Auto-ignition
NH3
H2
Crank angle (°CA ATDC)
X_{NH3}=1.0 X_{NH3}=0.9
X_{NH3}=0.7 X_{NH3}=0.5



NO (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0 X_{NH3}=0.9
X_{NH3}=0.7 X_{NH3}=0.5
CAHEMA



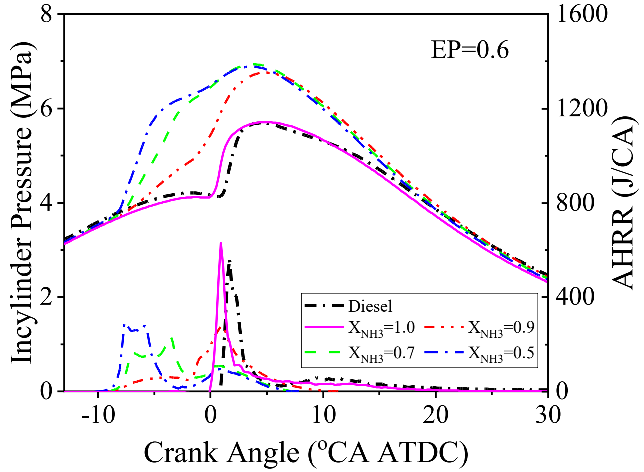
N2O (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0 X_{NH3}=0.9
X_{NH3}=0.7 X_{NH3}=0.5

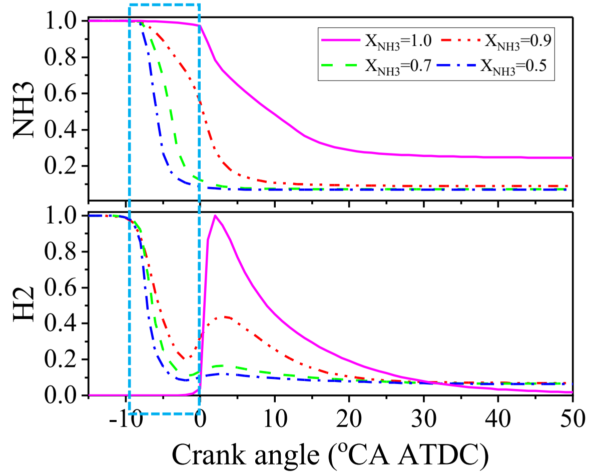


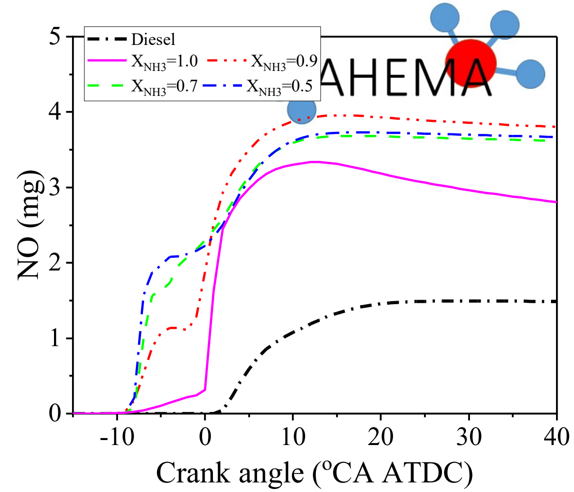
NO2 (mg)
Crank angle (°CA ATDC)
Diesel
X_{NH3}=1.0 X_{NH3}=0.9
X_{NH3}=0.7 X_{NH3}=0.5

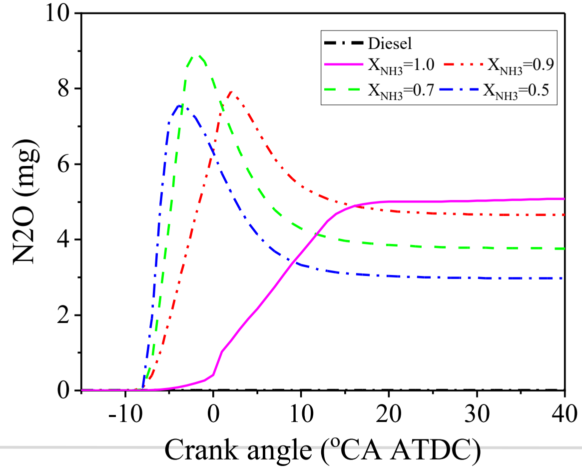
EP=0.6

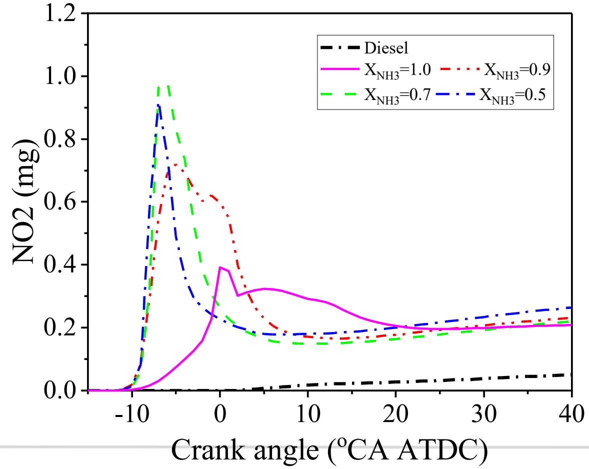
Auto-ignition



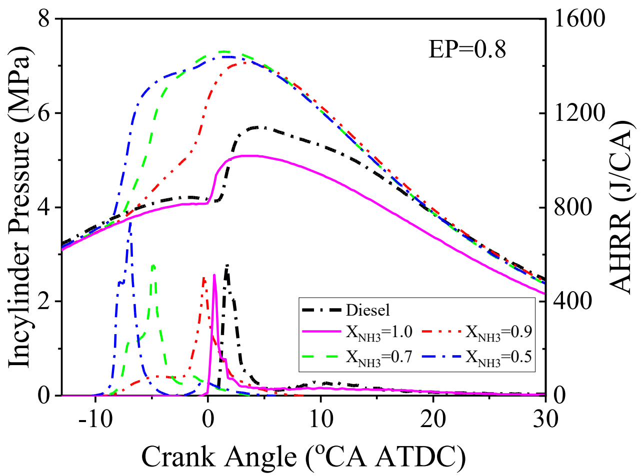


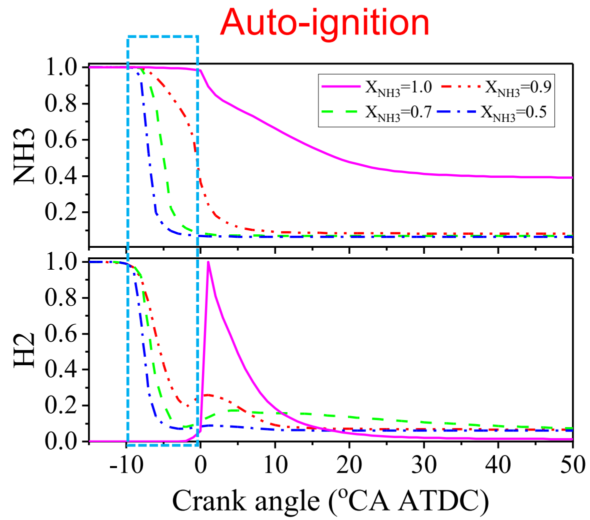


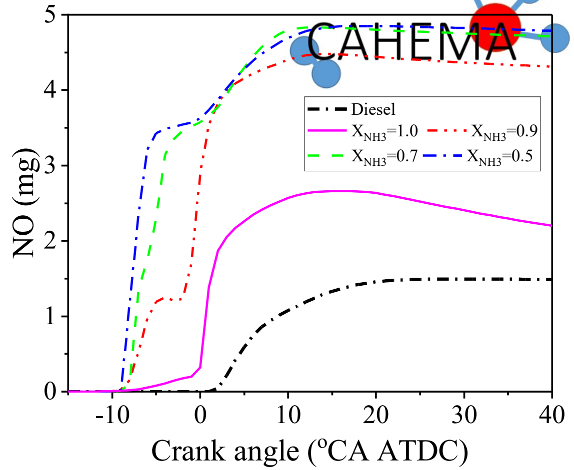


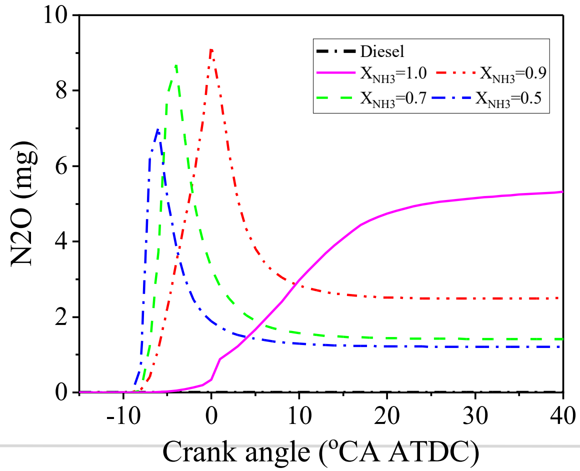


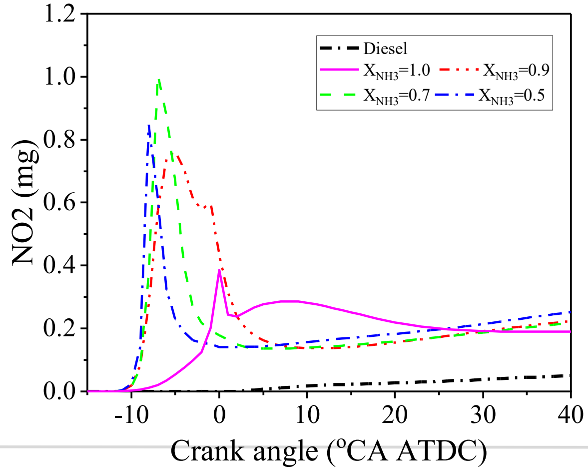
EP=0.8


EP=0.8
Incylinder Pressure (MPa)
AHRR (J/CA)
Crank Angle (°CA ATDC)
Diesel
X_NH3=1.0
X_NH3=0.9
X_NH3=0.7
X_NH3=0.5


Auto-ignition
NH3
H2
Crank angle (°CA ATDC)
X_NH3=1.0
X_NH3=0.9
X_NH3=0.7
X_NH3=0.5


NO (mg)
Crank angle (°CA ATDC)
Diesel
X_NH3=1.0
X_NH3=0.9
X_NH3=0.7
X_NH3=0.5


N2O (mg)
Crank angle (°CA ATDC)
Diesel
X_NH3=1.0
X_NH3=0.9
X_NH3=0.7
X_NH3=0.5

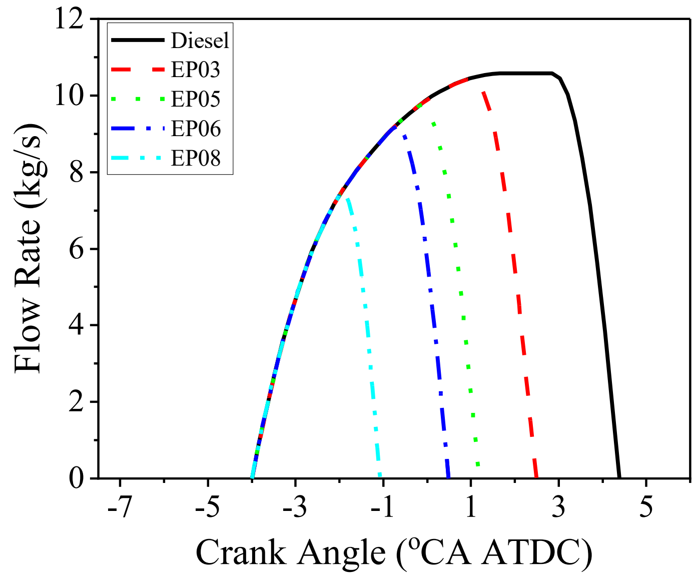

NO2 (mg)
Crank angle (°CA ATDC)
Diesel
X_NH3=1.0
X_NH3=0.9
X_NH3=0.7
X_NH3=0.5

NH3 RCCI engine (Medium load)

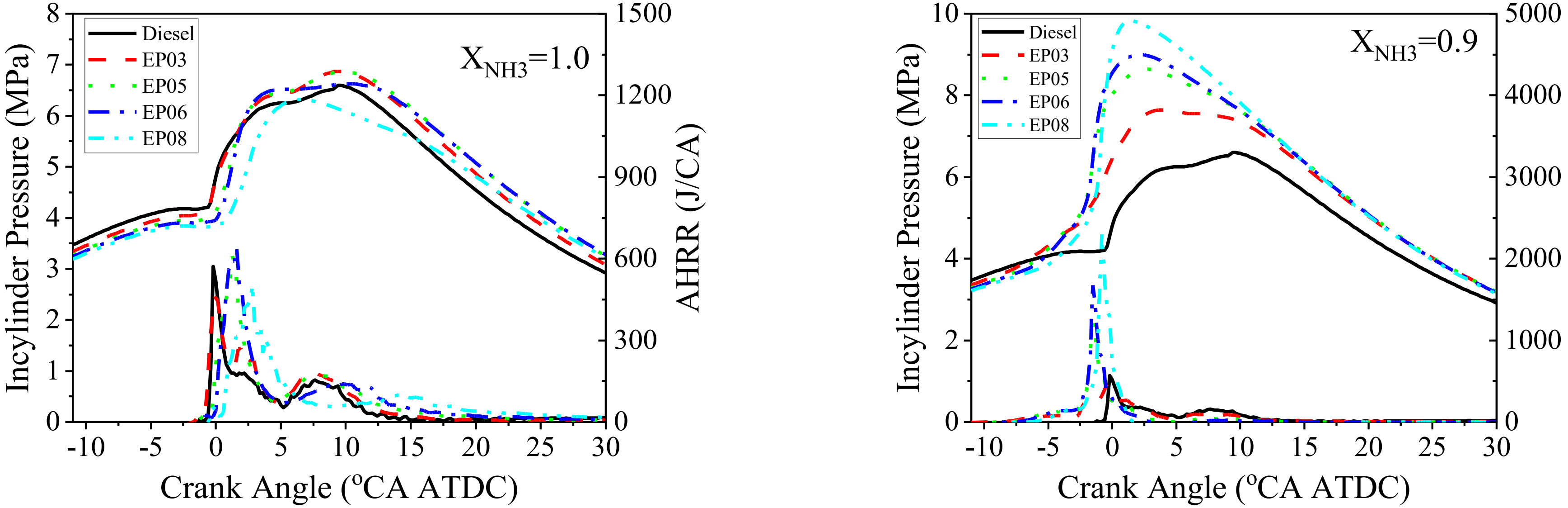
Medium load:

Total energy in the cylinder: 5000 J/cyc, IMEP 10bar

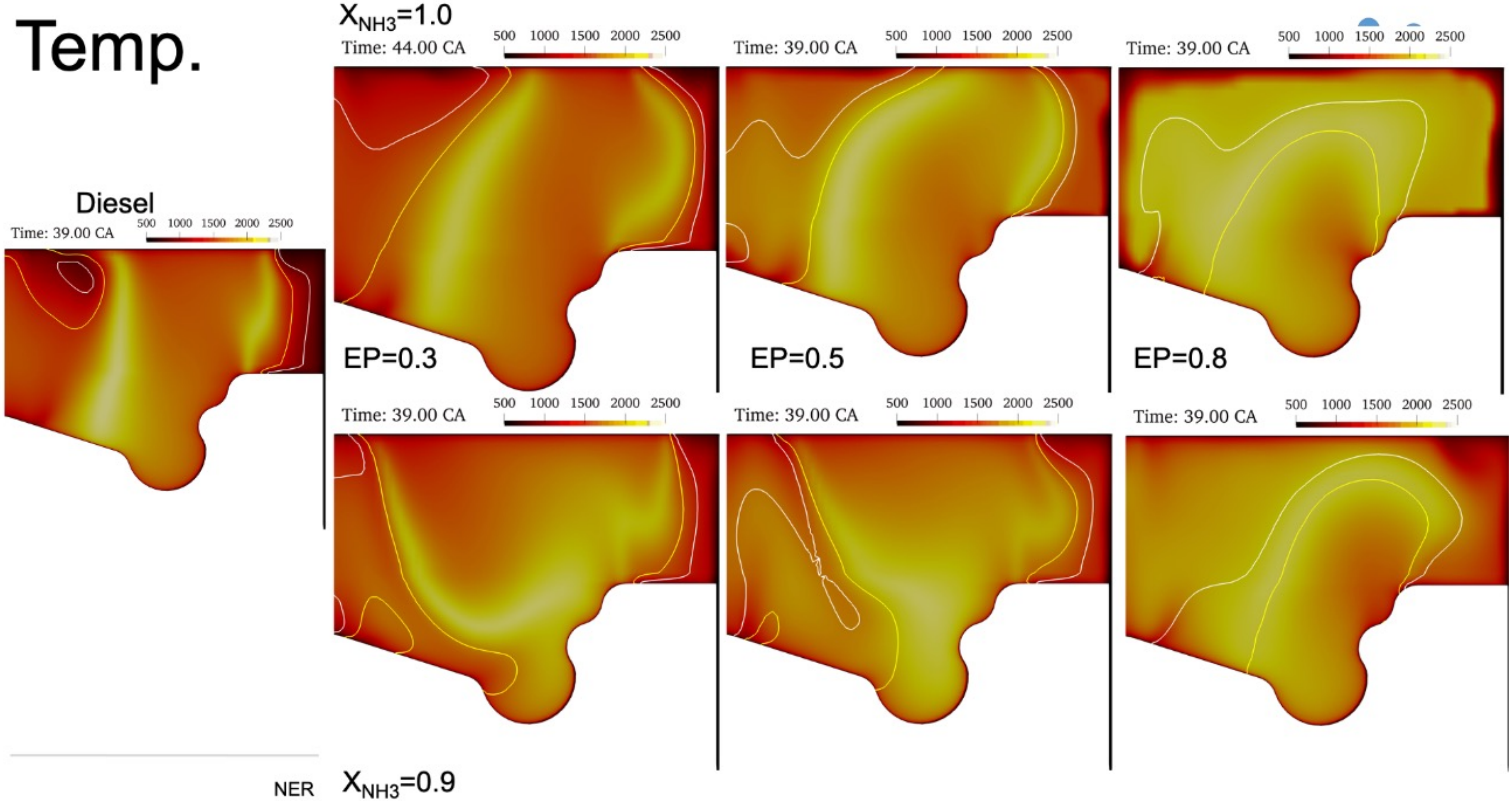
Case Name	EP	X_{NH3}	Φ_0 (premix)	Injected Duration °CA (N-heptane)	Description
Diesel	0	0	0	8.393	Diesel Engine
EP03	0.3	1	0.265	6.494	RCCI engine NH3 premixed
EP05	0.5		0.442	5.184	
EP06	0.6		0.530	4.493	
EP08	0.8		0.707	2.923	
NH3/H2 mixture premixed					
EP03	0.3	0.9	0.263	6.494	NH3/H2 premixed
EP05	0.5		0.438	5.184	
EP06	0.6		0.525	4.493	
EP08	0.8		0.701	2.923	



Engine performance

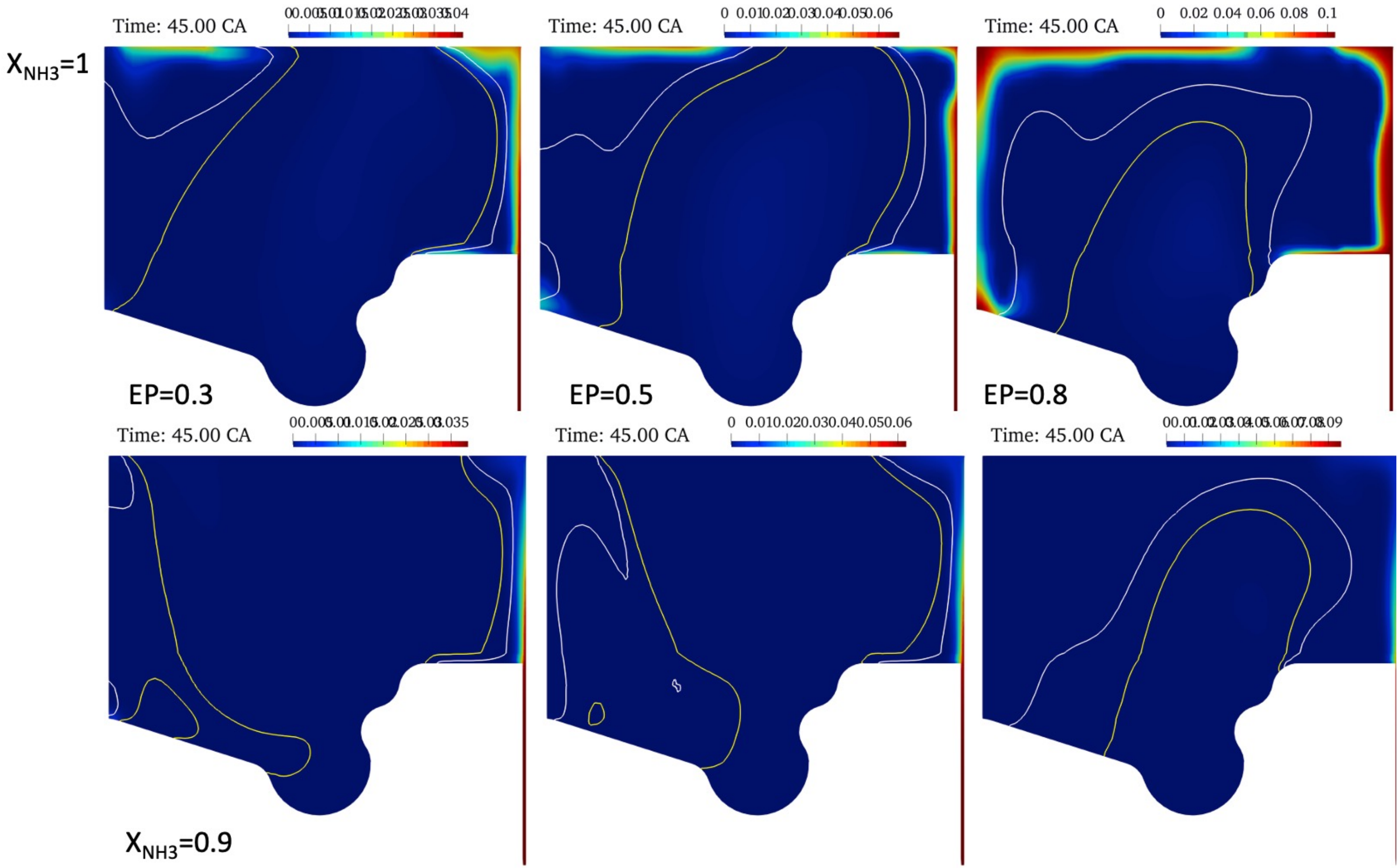


Temp.

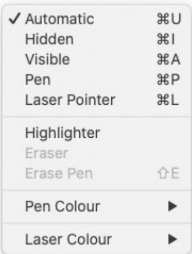


X_{NH3}=1.0
Diesel
Time: 39.00 CA
Time: 44.00 CA
Time: 39.00 CA
Time: 39.00 CA
500 1000 1500 2000 2500
EP=0.3
EP=0.5
EP=0.8
Time: 39.00 CA
Time: 39.00 CA
Time: 39.00 CA
NER
X_{NH3}=0.9

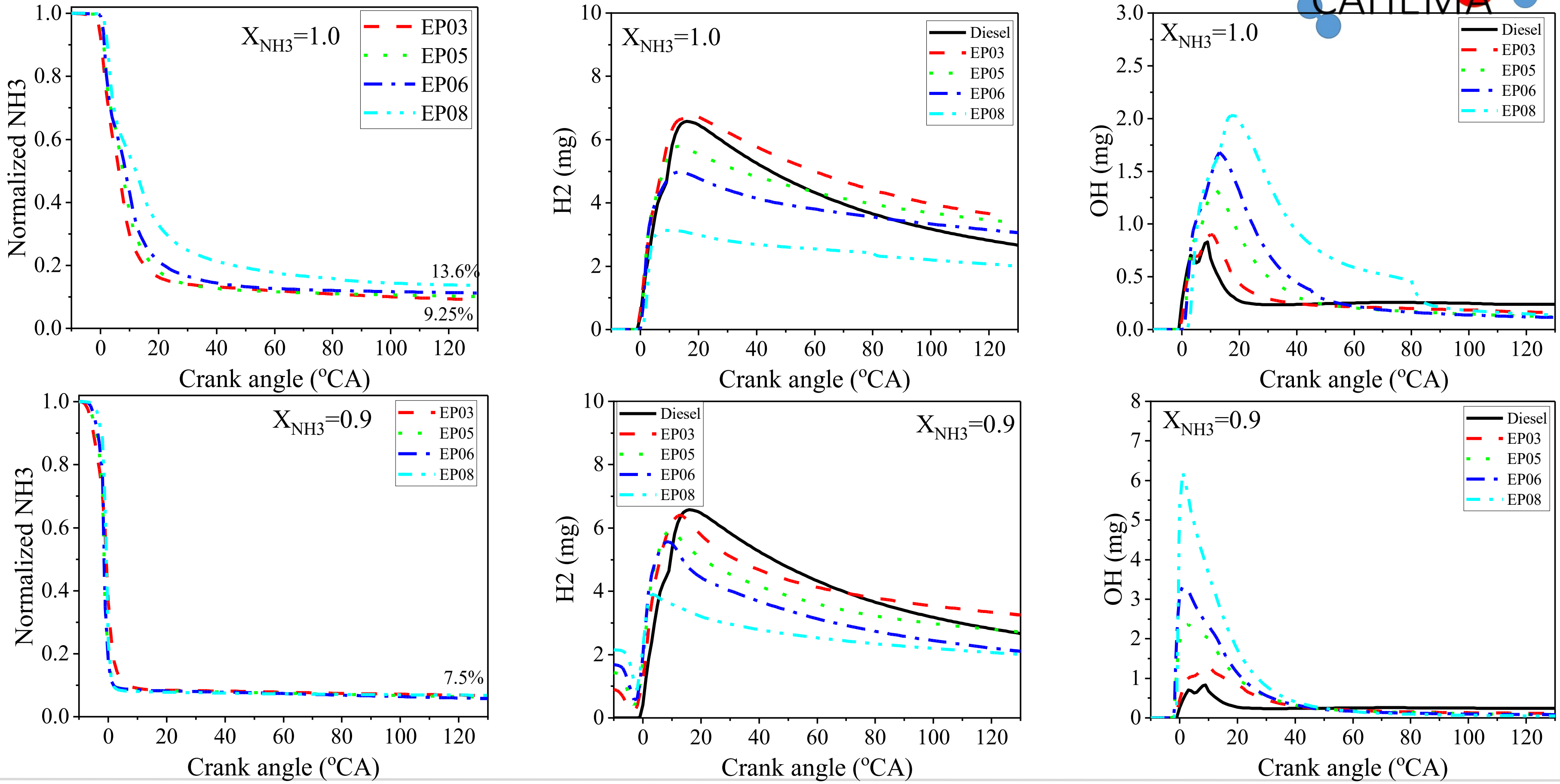
NH3



$X_{NH3}=1$
Time: 45.00 CA
EP=0.3
EP=0.5
EP=0.8
0 0.02 0.04 0.06 0.08 0.1
$X_{NH3}=0.9$

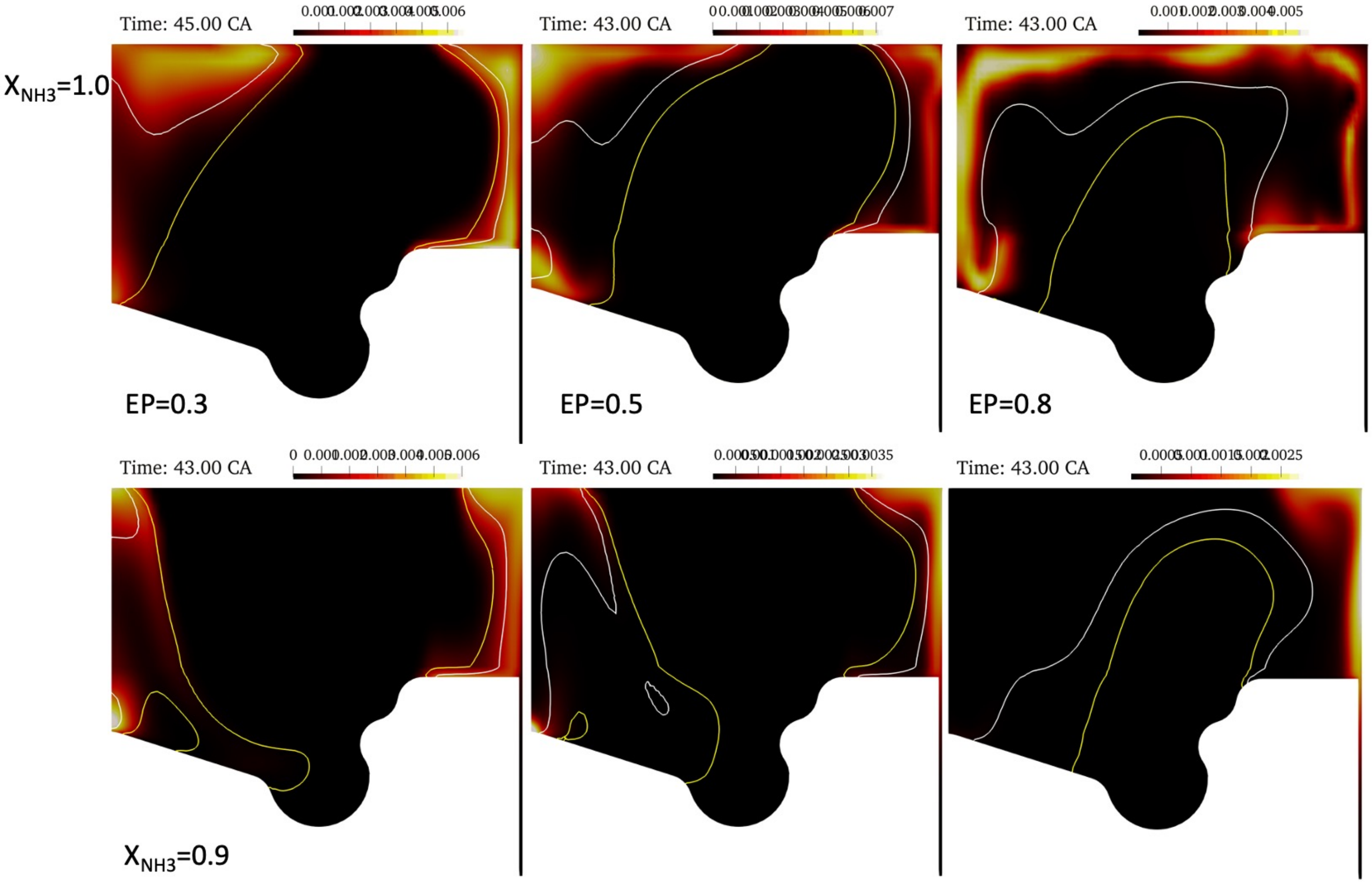


Automatic ⌘U
Hidden ⌘I
Visible ⌘A
Pen ⌘P
Laser Pointer ⌘L
Highlighter
Eraser
Erase Pen ⇧E
Pen Colour
Laser Colour

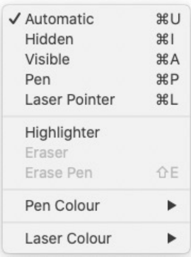


X_{NH3}=1.0
EP03
EP05
EP06
EP08
13.6%
9.25%
Normalized NH3
Crank angle (°CA)
H2 (mg)
Diesel
OH (mg)
X_{NH3}=0.9
7.5%

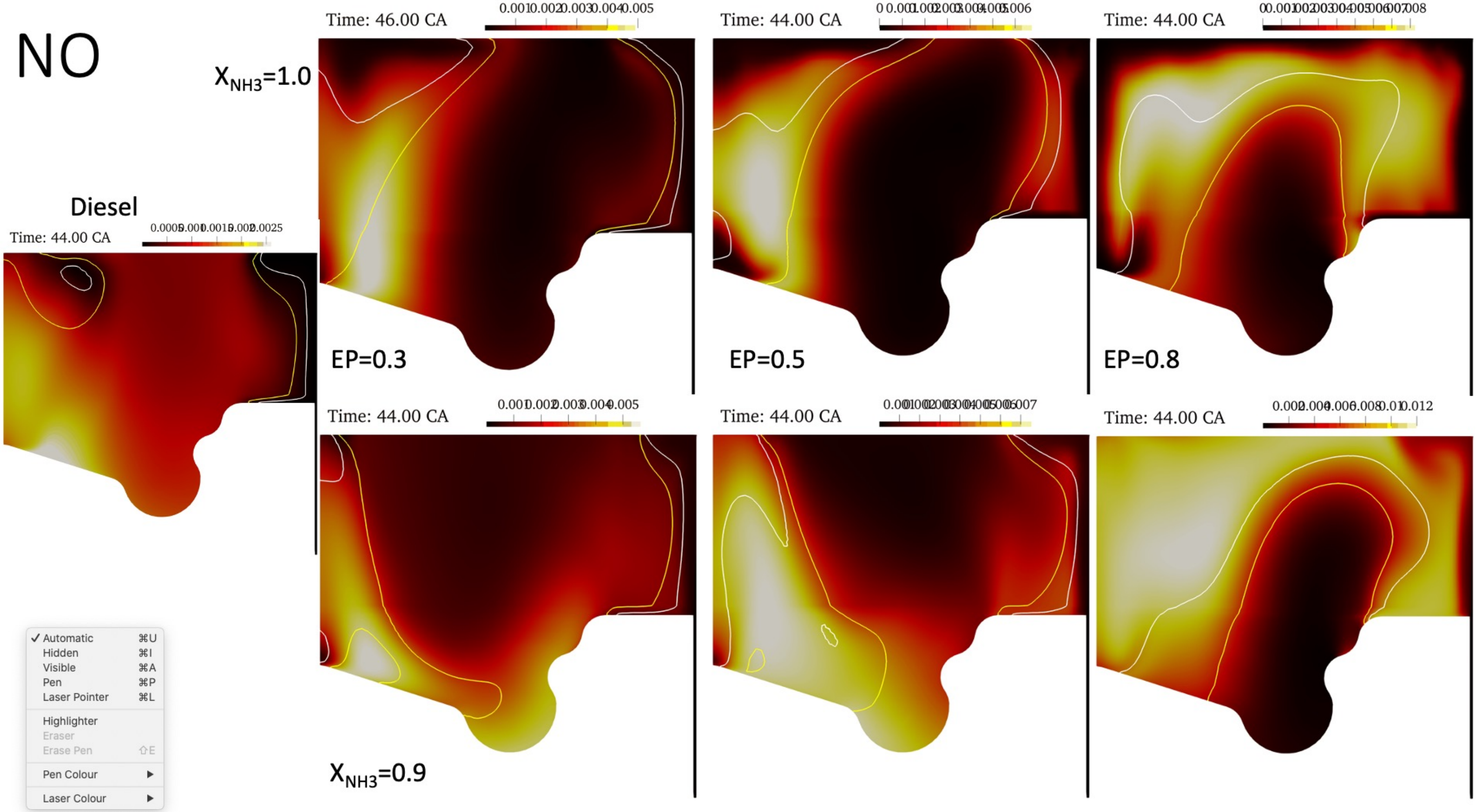
N2O

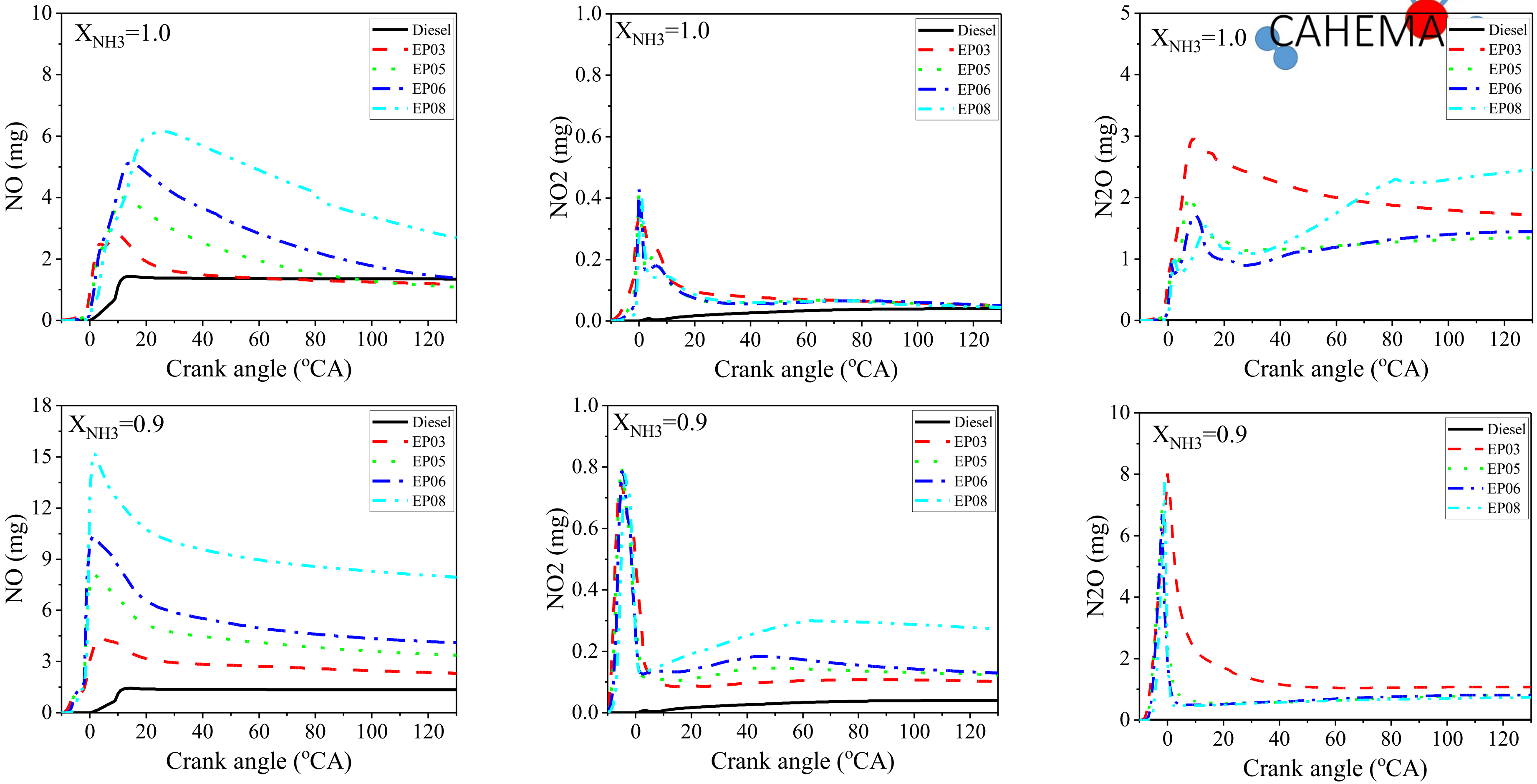


X_{NH3}=1.0
Time: 45.00 CA
Time: 43.00 CA
Time: 43.00 CA
EP=0.3
EP=0.5
EP=0.8
Time: 43.00 CA
Time: 43.00 CA
Time: 43.00 CA
X_{NH3}=0.9



✓ Automatic ⌘U
Hidden ⌘I
Visible ⌘A
Pen ⌘P
Laser Pointer ⌘L
Highlighter
Eraser
Erase Pen ⇧E
Pen Colour ▶
Laser Colour ▶


NO
Diesel
Time: 44.00 CA
X_{NH3}=1.0
Time: 46.00 CA
Time: 44.00 CA
Time: 44.00 CA
EP=0.3
EP=0.5
EP=0.8
Time: 44.00 CA
Time: 44.00 CA
Time: 44.00 CA
X_{NH3}=0.9
Automatic
Hidden
Visible
Pen
Laser Pointer
Highlighter
Eraser
Erase Pen
Pen Colour
Laser Colour


XNH3=1.0
NO (mg)
NO2 (mg)
N2O (mg)
XNH3=0.9
Crank angle (oCA)
Diesel
EP03
EP05
EP06
EP08

NH3 RCCI engine (high load)

High load: total energy in the cylinder: 7500 J/cyc, IMEP 15bar

The global Φ~1.3， Thus, increasing the intake pressure (**supercharging**)

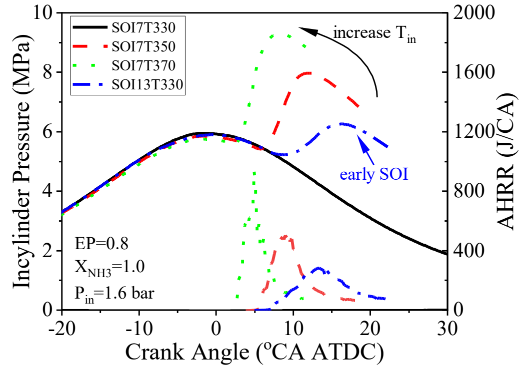
Intake pressure：1.2 bar → 1.6 bar
T_{in}： 458K → 330K

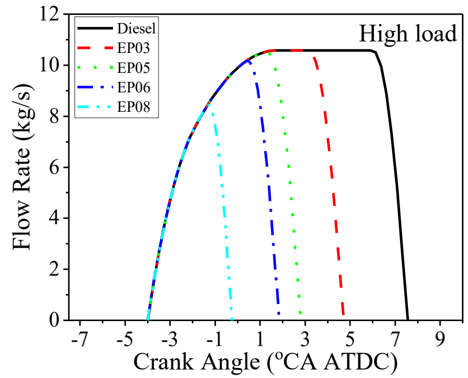
→ Increase the mass of intake air

SOI：-7 °CA ATDC → -13 °CA ATDC

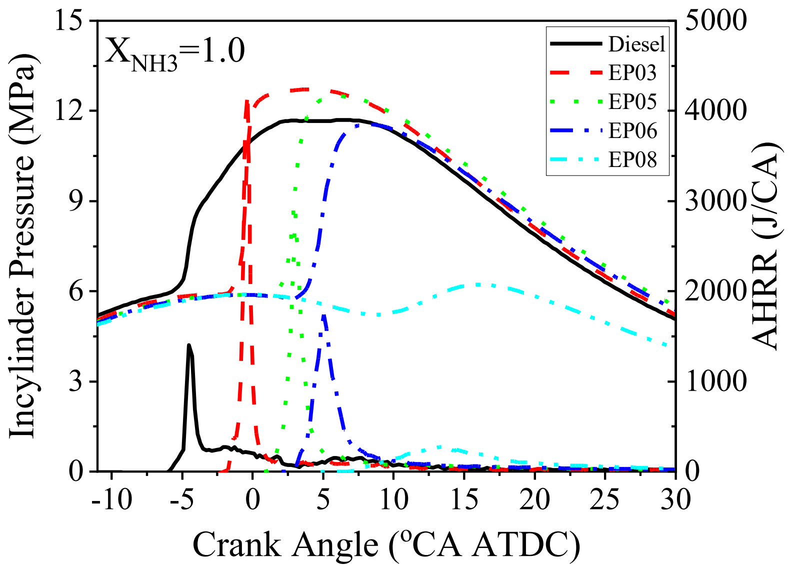
→ Promote the ignition of diesel

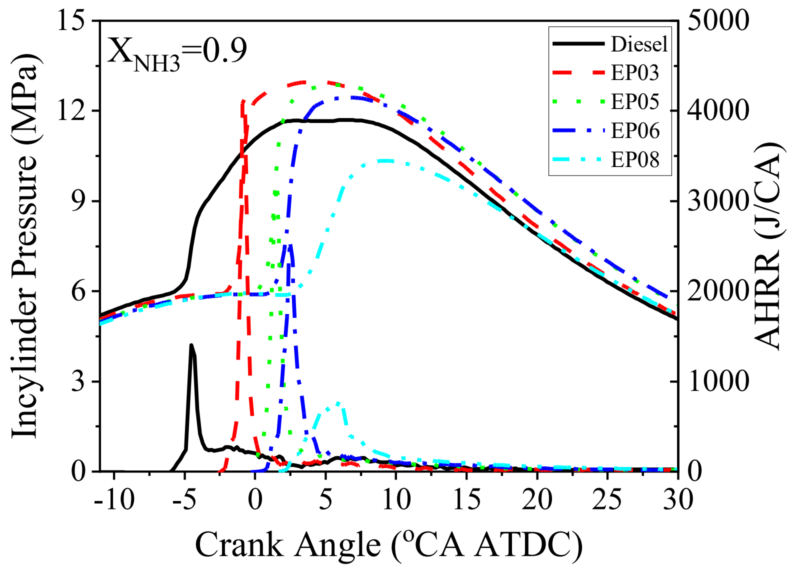
Case Name	EP	X_{NH3}	Φ_0 (premix)	Injected Duration °CA (N-heptane)	Description
Diesel	0	0	**0**	11.556	Diesel Engine
EP03	0.3	1	**0.209**	8.712	RCCI engine NH3 premixed
EP05	0.5		**0.348**	6.811	
EP06	0.6		**0.418**	5.846	
EP08	0.8		**0.557**	3.751	
NH3/H2 mixture premixed					
EP03	0.3	0.9	**0.207**	6.494	NH3/H2 premixed
EP05	0.5		**0.345**	5.184	
EP06	0.6		**0.414**	4.493	
EP08	0.8		**0.552**	2.923	



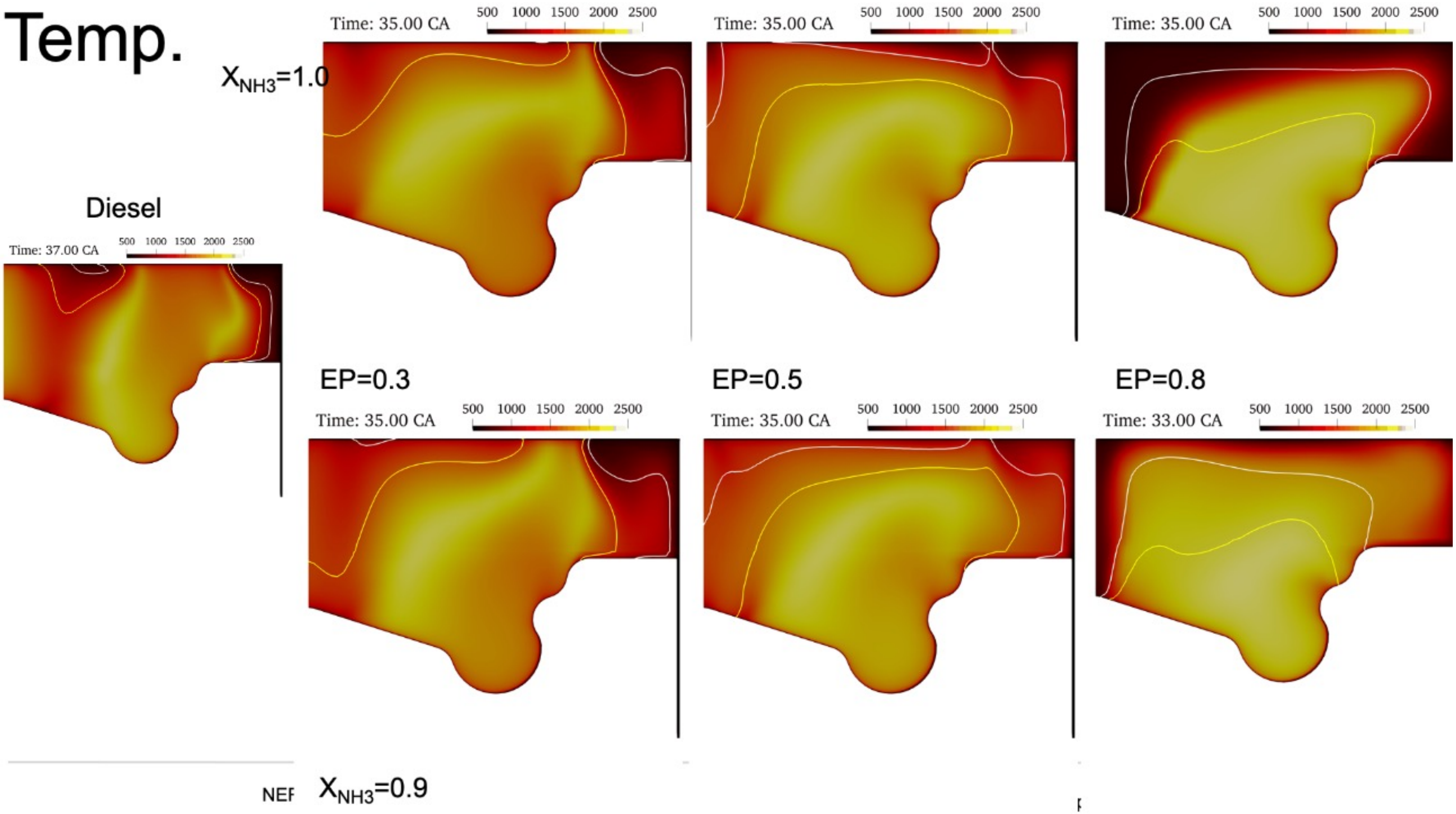


Engine performance

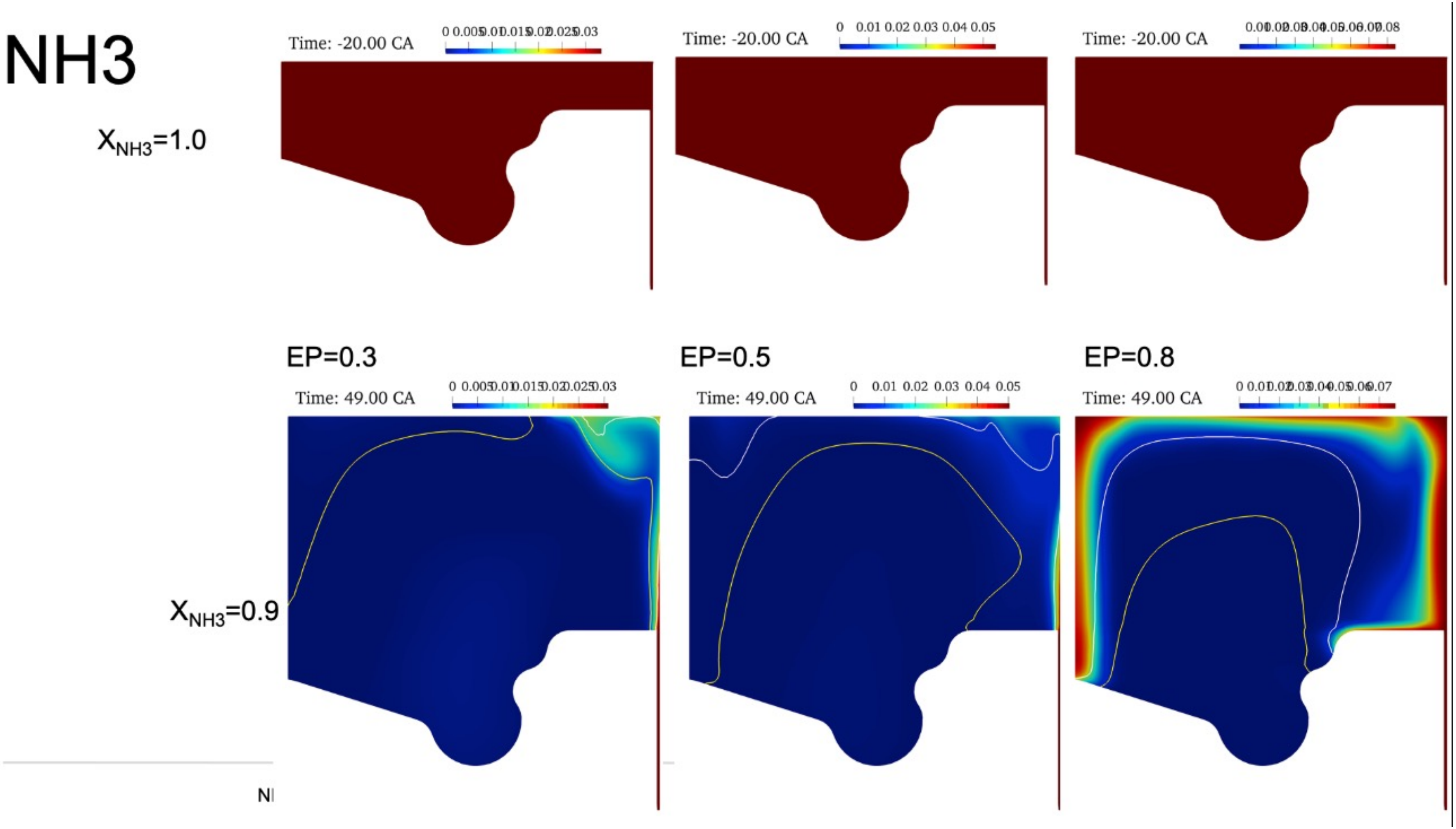


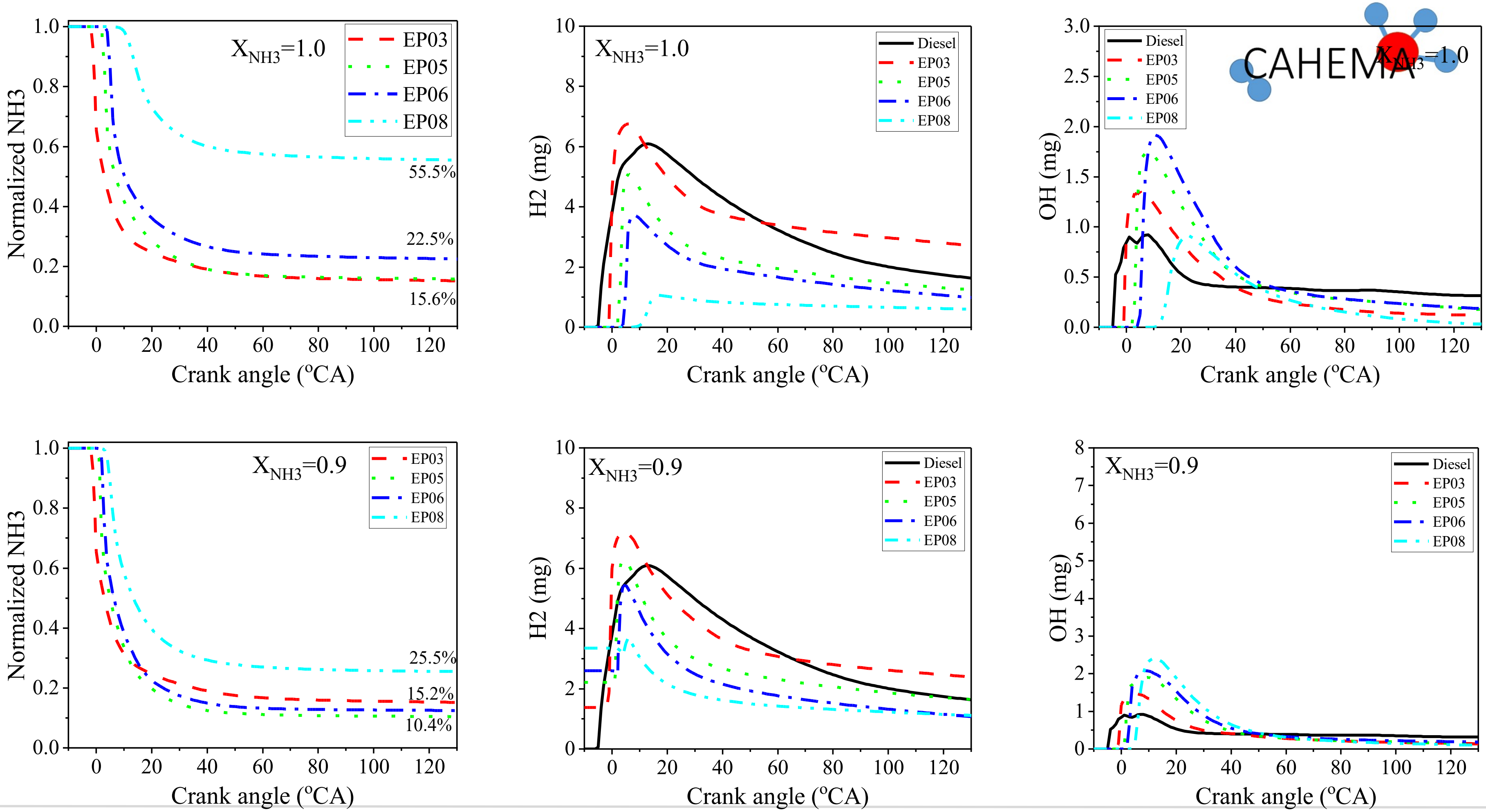


Temp.



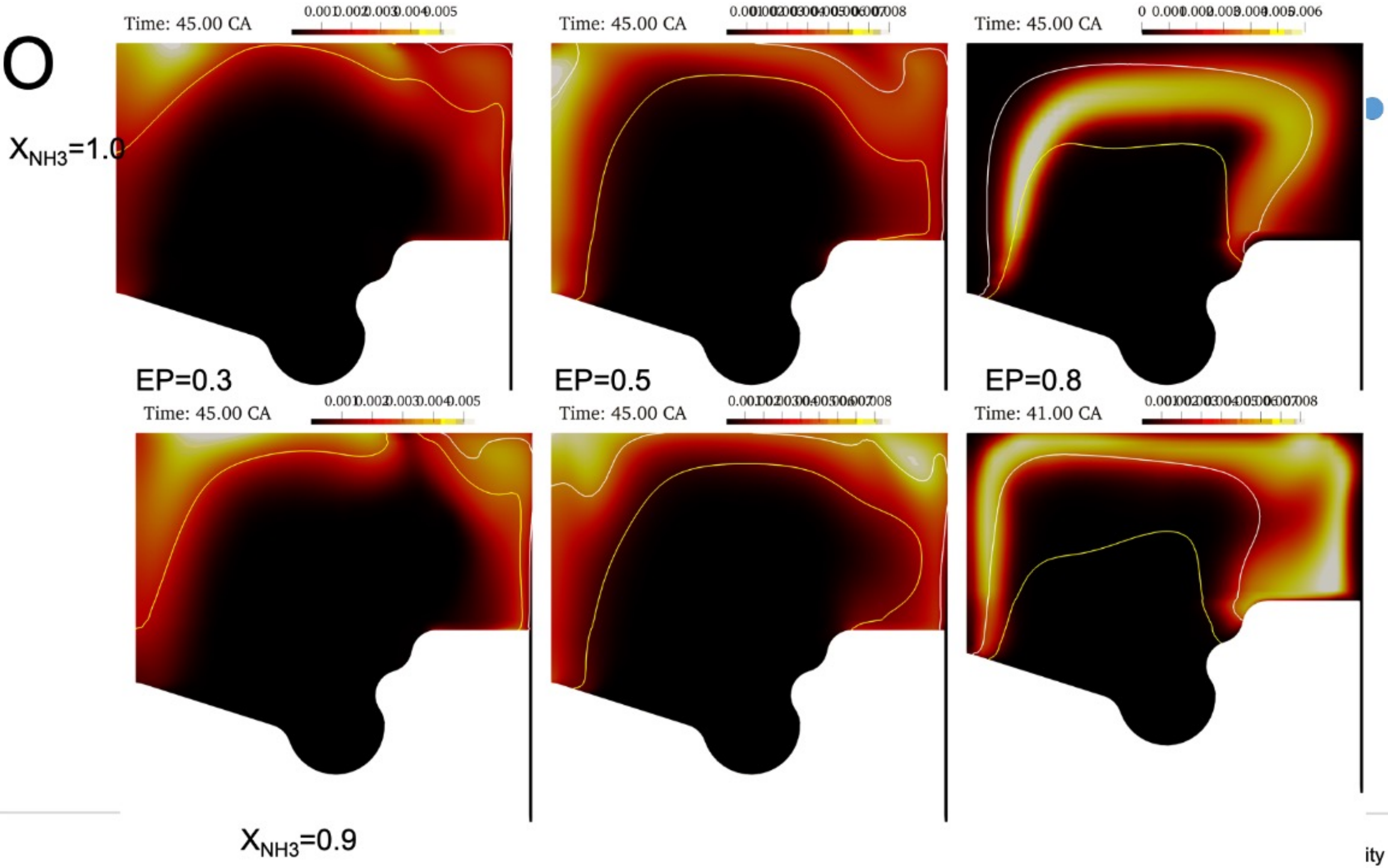
Diesel
Time: 37.00 CA
500 1000 1500 2000 2500
X_{NH3}=1.0
Time: 35.00 CA
500 1000 1500 2000 2500
Time: 35.00 CA
500 1000 1500 2000 2500
Time: 35.00 CA
500 1000 1500 2000 2500
EP=0.3
EP=0.5
EP=0.8
Time: 35.00 CA
500 1000 1500 2000 2500
Time: 35.00 CA
500 1000 1500 2000 2500
Time: 33.00 CA
500 1000 1500 2000 2500
X_{NH3}=0.9


NH3
X_NH3=1.0
Time: -20.00 CA
Time: -20.00 CA
Time: -20.00 CA
0 0.01 0.02 0.03 0.04 0.05
EP=0.3
EP=0.5
EP=0.8
Time: 49.00 CA
Time: 49.00 CA
Time: 49.00 CA
0 0.01 0.02 0.03 0.04 0.05
X_NH3=0.9



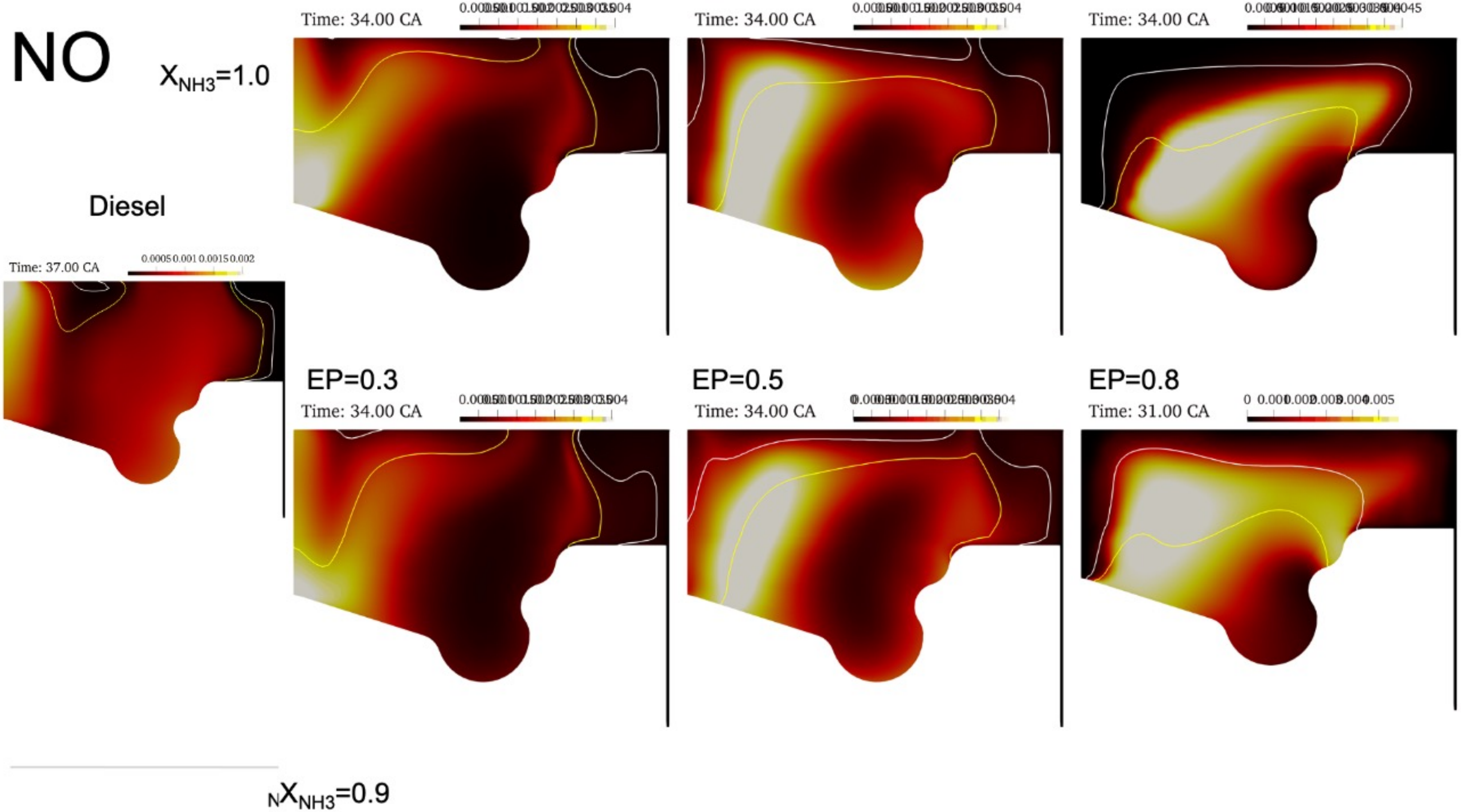
X_{NH3}=1.0
EP03
EP05
EP06
EP08
55.5%
22.5%
15.6%
Normalized NH3
Crank angle (°CA)
X_{NH3}=1.0
Diesel
EP03
EP05
EP06
EP08
H2 (mg)
Crank angle (°CA)
X_{NH3}=1.0
Diesel
EP03
EP05
EP06
EP08
OH (mg)
Crank angle (°CA)
X_{NH3}=0.9
EP03
EP05
EP06
EP08
25.5%
15.2%
10.4%
Normalized NH3
Crank angle (°CA)
X_{NH3}=0.9
Diesel
EP03
EP05
EP06
EP08
H2 (mg)
Crank angle (°CA)
X_{NH3}=0.9
Diesel
EP03
EP05
EP06
EP08
OH (mg)
Crank angle (°CA)

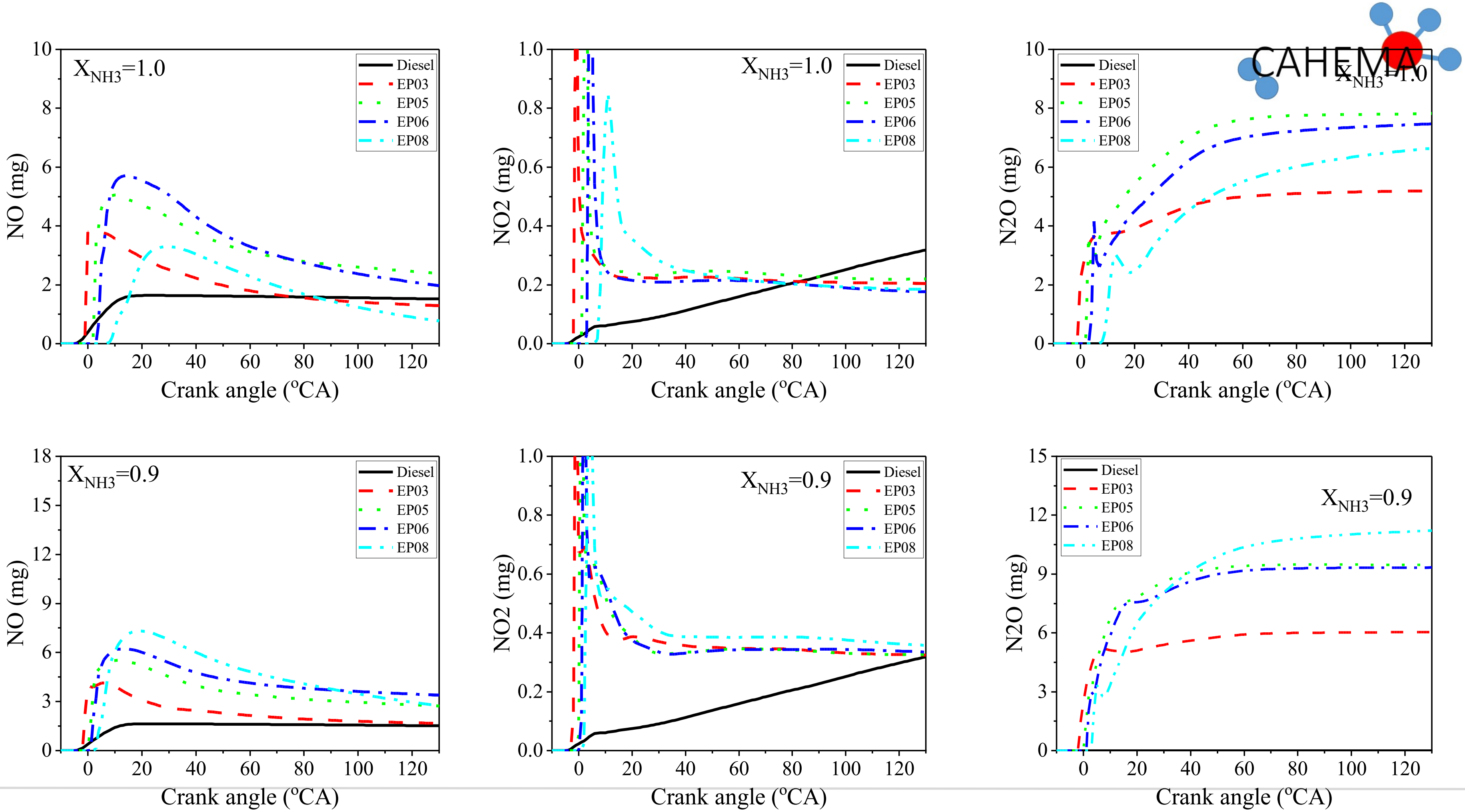
N2O



X_{NH3}=1.0
Time: 45.00 CA
Time: 45.00 CA
Time: 45.00 CA
EP=0.3
EP=0.5
EP=0.8
Time: 45.00 CA
Time: 45.00 CA
Time: 41.00 CA
X_{NH3}=0.9

ity


NO
X_NH3=1.0
Diesel
Time: 37.00 CA
0.0005 0.001 0.0015 0.002
Time: 34.00 CA
Time: 34.00 CA
Time: 34.00 CA
EP=0.3
EP=0.5
EP=0.8
Time: 34.00 CA
Time: 34.00 CA
Time: 31.00 CA
NX_NH3=0.9


X_{NH3}=1.0
NO (mg)
NO2 (mg)
N2O (mg)
X_{NH3}=0.9
Crank angle (°CA)
Diesel
EP03
EP05
EP06
EP08
CAHEMA

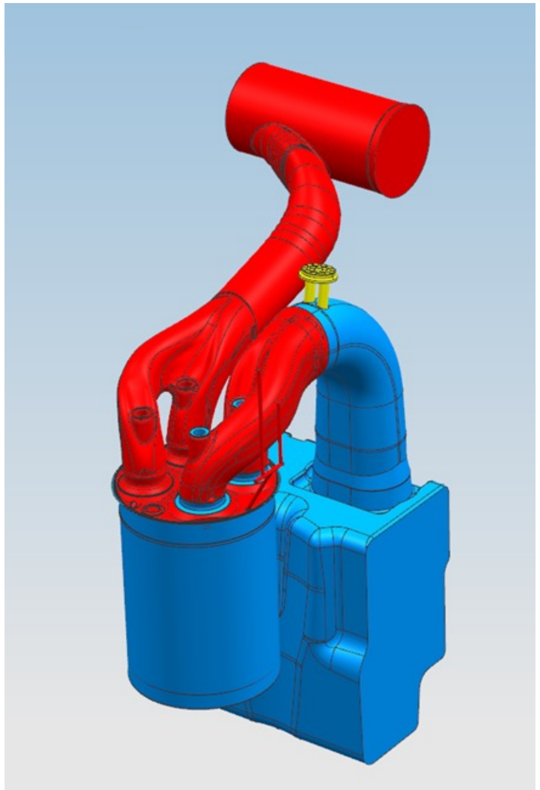
Summary and future work

- LES of n-heptane/ammonia RCCI ignition
  - Fuel chemistry interaction – suppression of auto-ignition
  - NO and N_2O flame structures
- CFD simulation of diesel/ammonia/hydrogen RCCI engine performed
  - Baseline engine tested for gasoline and methanol
  - Engine performance simulated
    - Three different loads
    - NH_3, NO, N_2O emissions
    - Effect of H2 on ammonia combustion
- Engine validation
  - NTNU/Aalto
  - Wärtsilä engine

Summary and future work

- CFD simulation of Wärtsilä four-stroke engine
  - Ongoing experiments at Wärtsilä
  - NDA signed
  - CFD meshing of engine geometry in progress
  - RCCI concept
  - DDFS concept

- CFD simulation of MAN two-stroke engine



Thank you for your support

PhD student
Mark Treacy (50%)

Researcher
Leilei Xu (50%)