



C I M E C

Desarrollos y aplicaciones de cálculo CFD para análisis y optimización de sistemas de combustión en motores

II Jornadas Iberoamericanas de Motores Térmicos y Lubricantes
29-31 Agosto, 2018
Santa Fe, Argentina



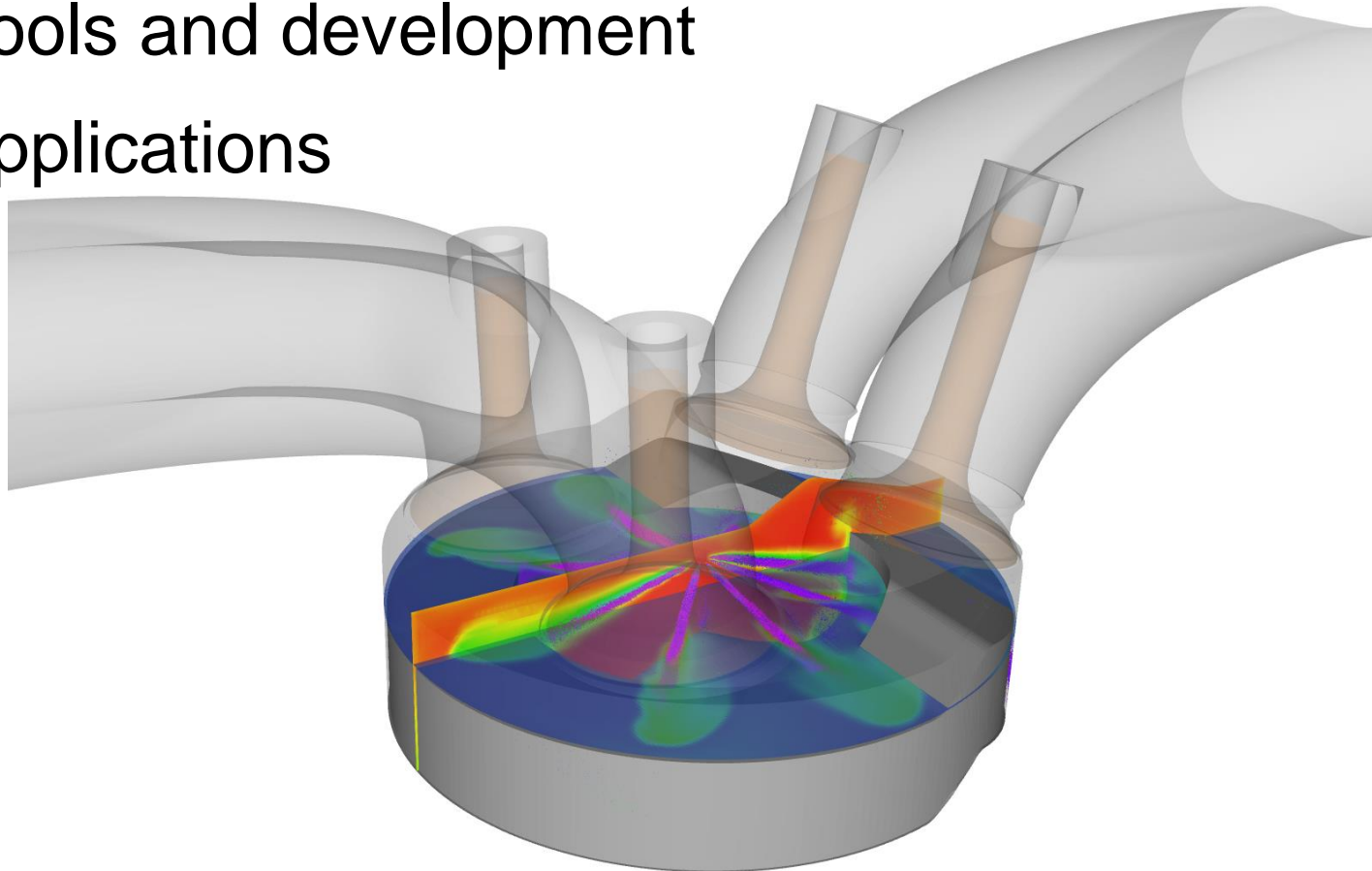
UNIVERSITAT
POLITÈCNICA
DE VALÈNCIA



José M. Pastor, Ph.D.

CONTENTS

- Background and approach
- Tools and development
- Applications

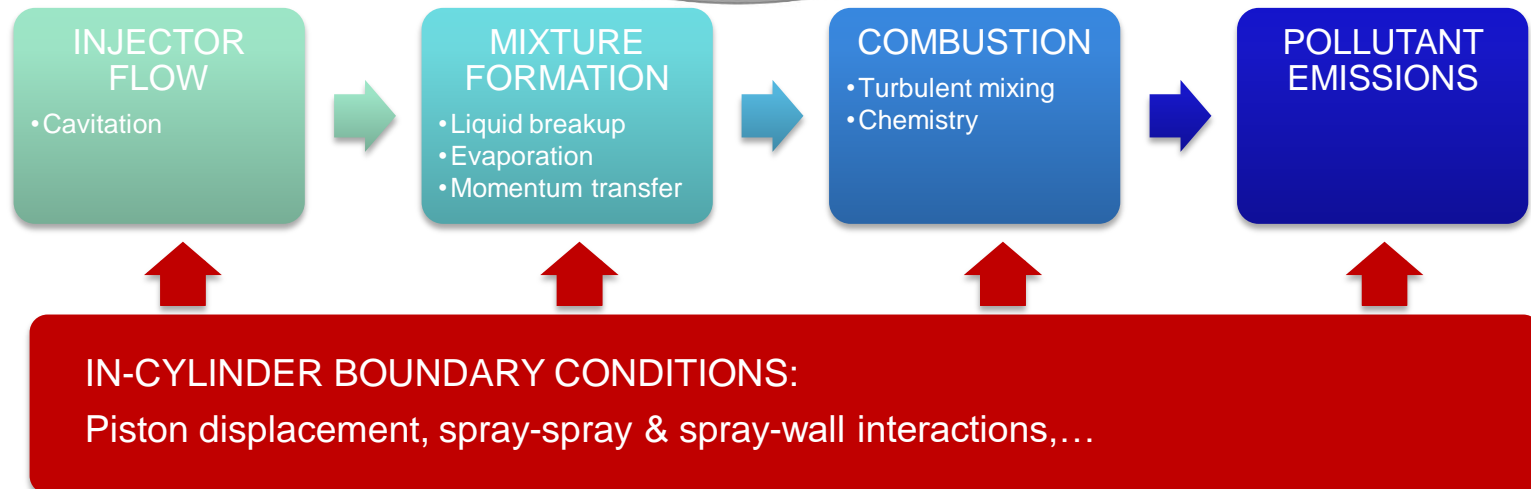
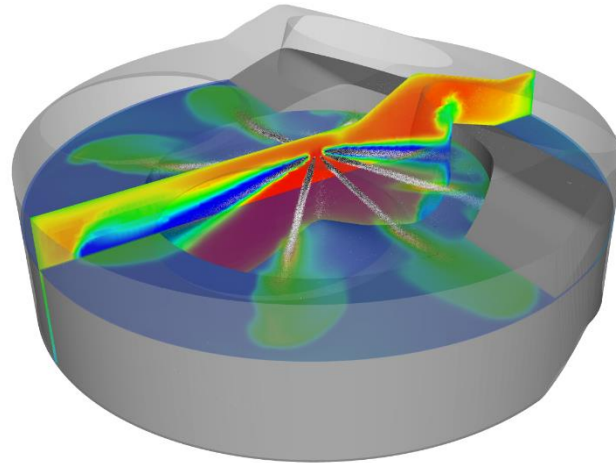


Motivation

- Energy conversion by combustion processes
 - Today about 80% of total primary energy supply (TPES) from fossil fuels
 - In 2035 TPES increases by 7%-29% with about 70% fossil fuels
 - Need for efficient combustion systems
 - ICEs are main power source in transportation sector
 - Increasingly stringent pollutant regulation for passenger cars and trucks
 - Demand on new low-consumption & pollutants aircraft engines
 - Design of combustion devices is challenging task
 - Complex multi-physics and chemical process
 - Development by means of experiments (empirical approach)
 - Support design process with simulation tools
 - Numerical models to improve understanding
- } Gaining attention
in the latest decades

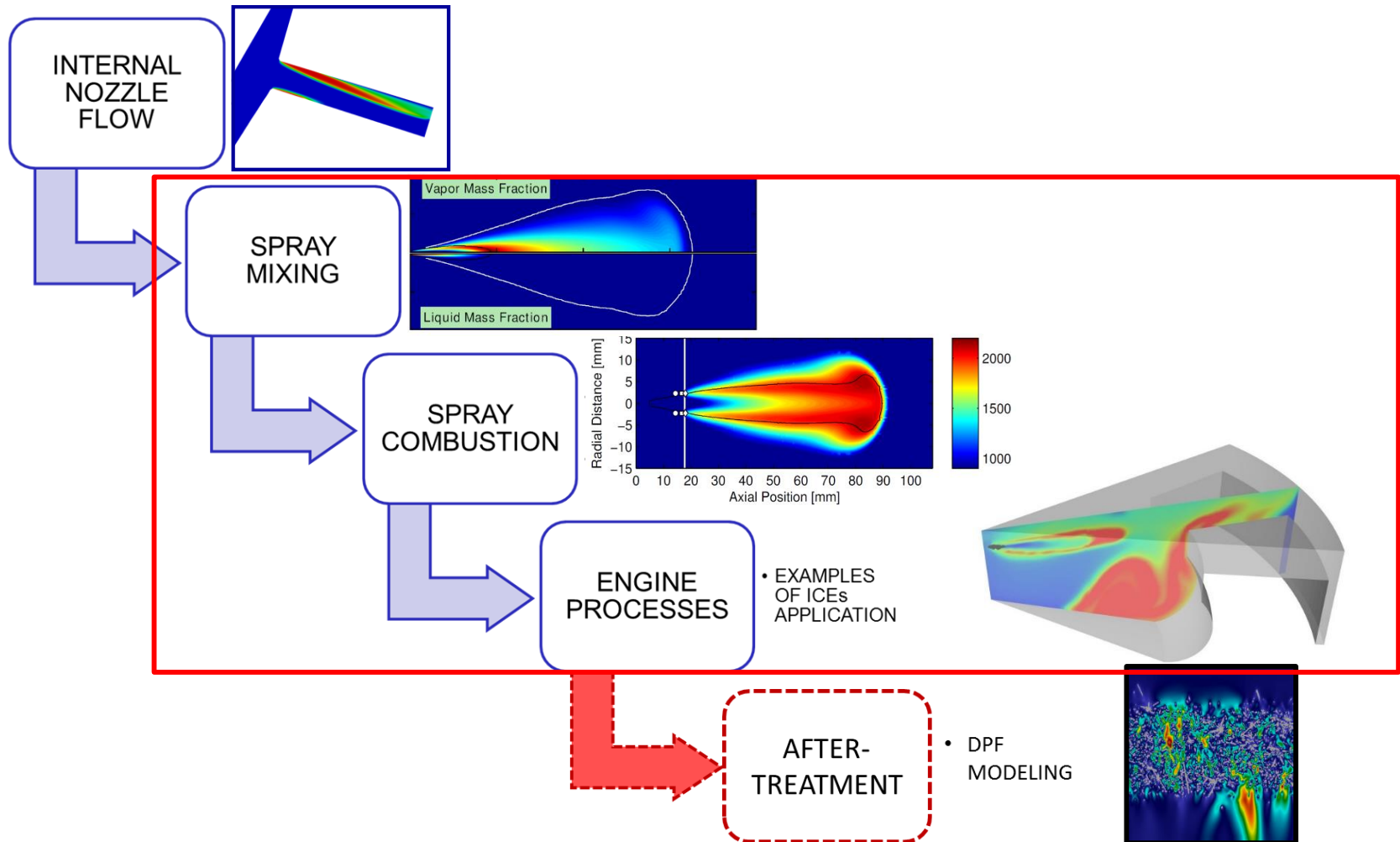
CFD of combustion in IC engines still a challenge:

- Complexity of the physical and chemical fundamental processes in a highly transient environment



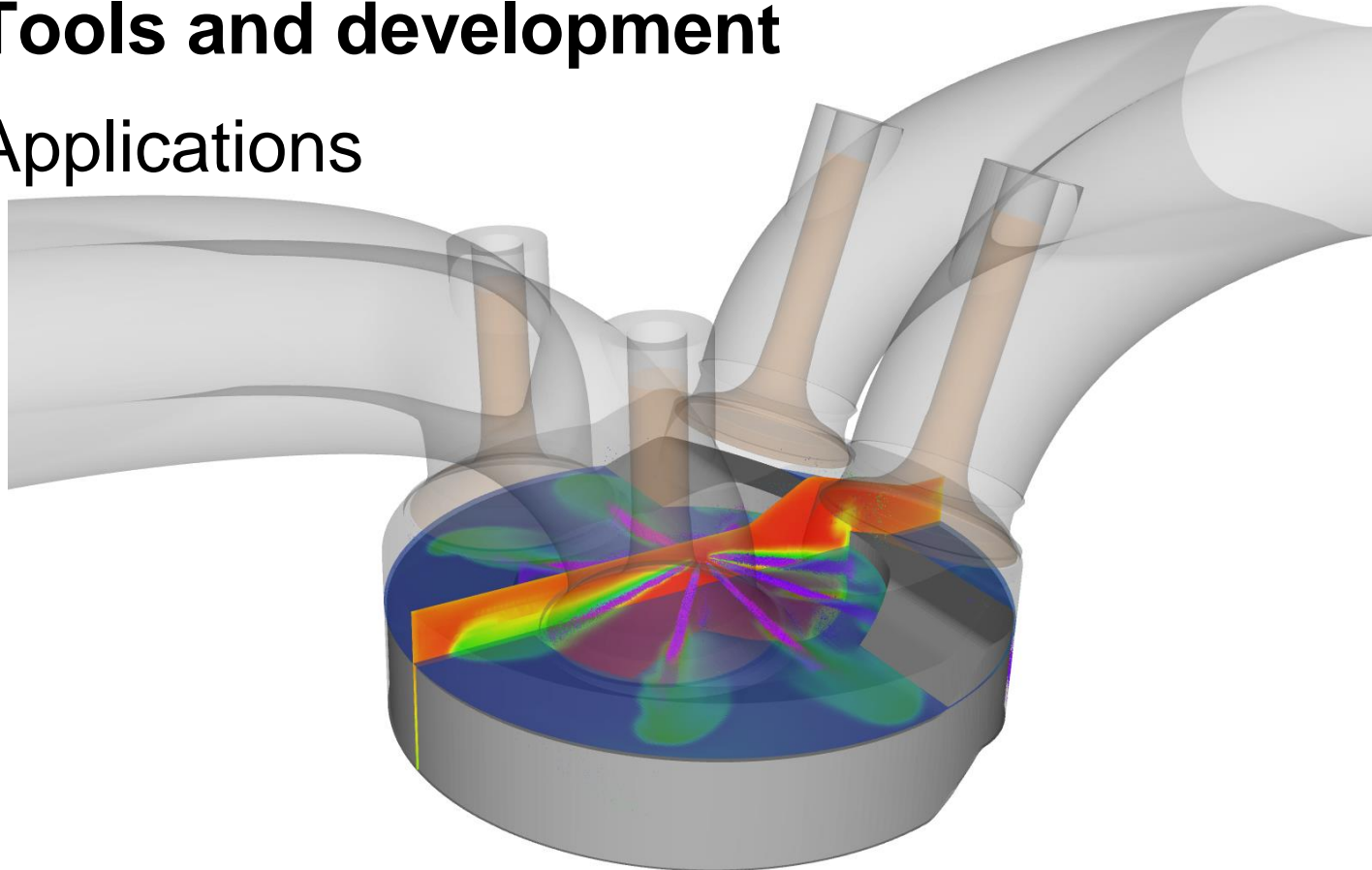
Modelling steps for RICEs CFD simulations

- Focused in Compression Ignited engines



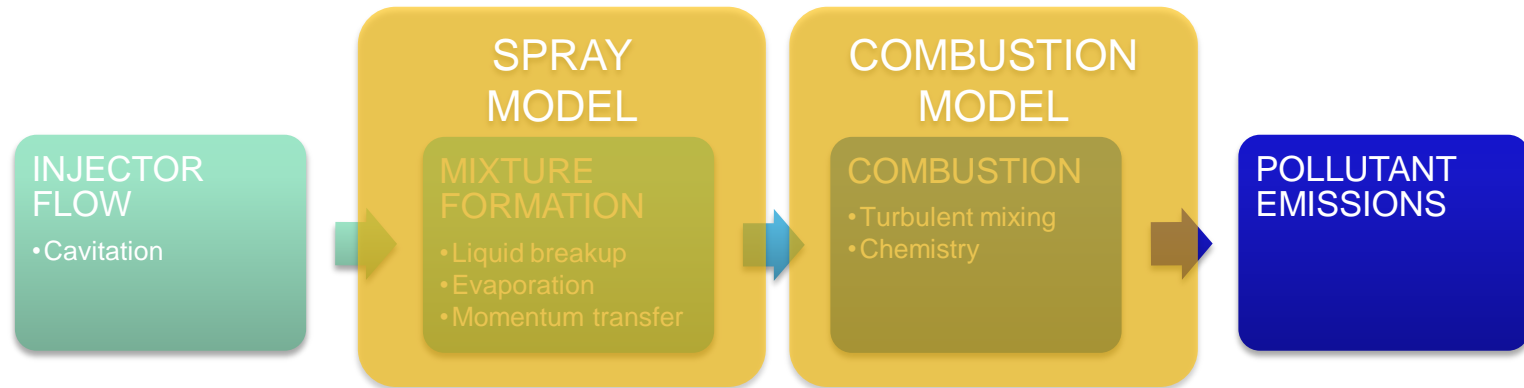
CONTENTS

- Background and approach
- **Tools and development**
- Applications



CFD of multiphase reacting flows

- State-of-the-art and research directions



	SPRAY	COMBUSTION	TURBULENCE
CONVENTIONAL	LAGRANGIAN (DDM)	SIMPLIFIED KINETICS + TCI	RANS
ADVANCED	EULERIAN +LAGRANGIAN	DETAILED KINETICS + TCI	RANS → LES

Engine Combustion Network (ECN)

- Necessary dialogue between research efforts

Experiments

Calculations

CRF Close collaboration and pathway to better CFD tools

Experiment	CFD codes used	CFD approaches	Modeling submissions
Sandia Mich. Techn.	CONVERGE	RANS	Sandia
Argonne Meiji	Star CD	LES	Argonne
IFPEN Infineum	Open FOAM	High-fidelity LES	IFPEN
CMT Chalmers	KIVA	Eulerian-Eulerian	CMT
CAT KAIST	ANSYS Fluent & CFX	Eulerian-Lagrangian	Polimi
GM Aachen	FORTE	Dense fluid	UMass
Delphi Melbourne	RAPTOR	many spray and combustion variants...	UNSW
Bosch Brighton	other research codes...		Penn St.
TU/e Michigan			TU/e
Ist. Motori			UW-Madison
			Purdue
			ETH-Zurich
			Aalto
			Aachen
			DTU
			Cambridge
			Georgia Tech
			Chalmers
			GM...

ECN organization

- Monthly web meetings
- Workshop organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review
- Very tight coordination because of target conditions

Most industry use ECN data to test their CFD practices

COMBUSTION RESEARCH FACILITY Sandia National Laboratories

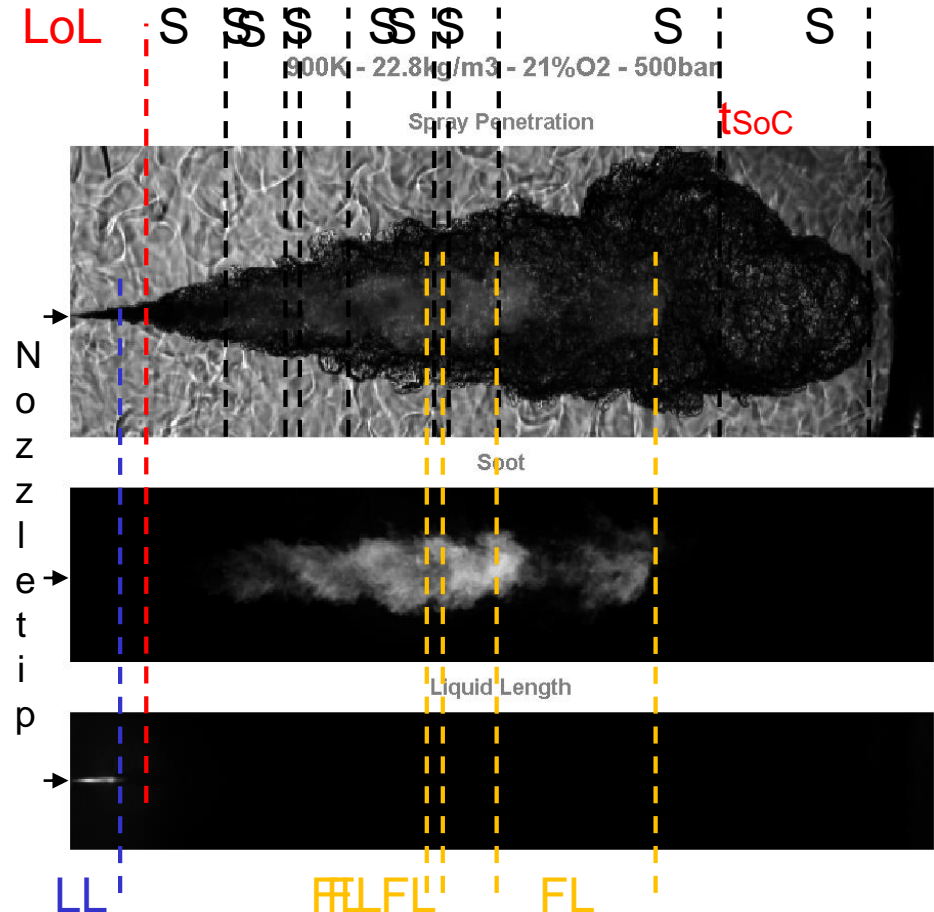
Diesel spray combustion, a highly transient process

■ Inert phase

- Tip penetration (S)
- Liquid stabilization (LL)

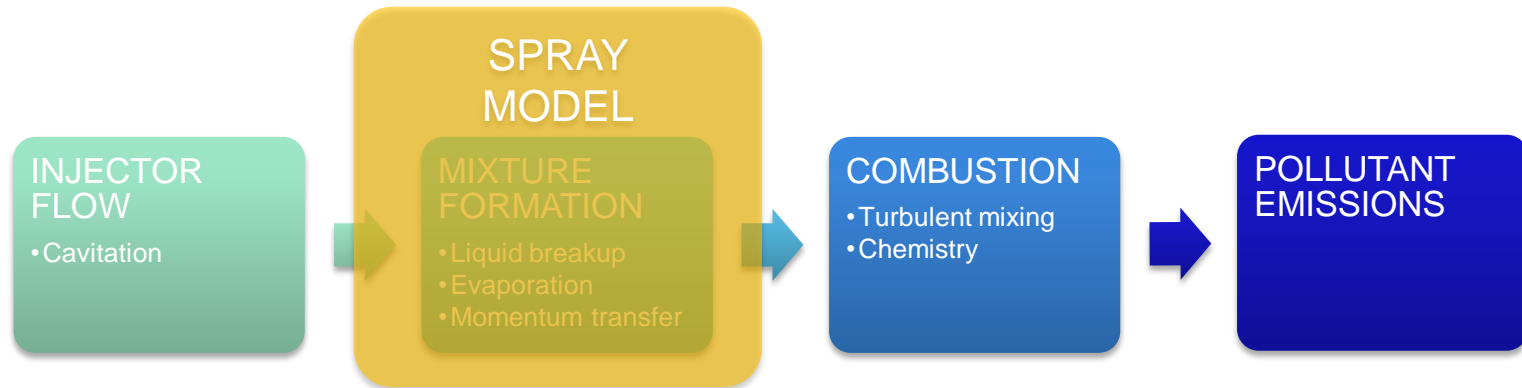
■ Auto-ignition and diffusion flame

- Tip penetration (S)
- Ignition delay (t_{SoC})
- Lift-off length (LOL)
- Flame stabilization (FL)



CFD of multiphase reacting flows

- State-of-the-art and research directions



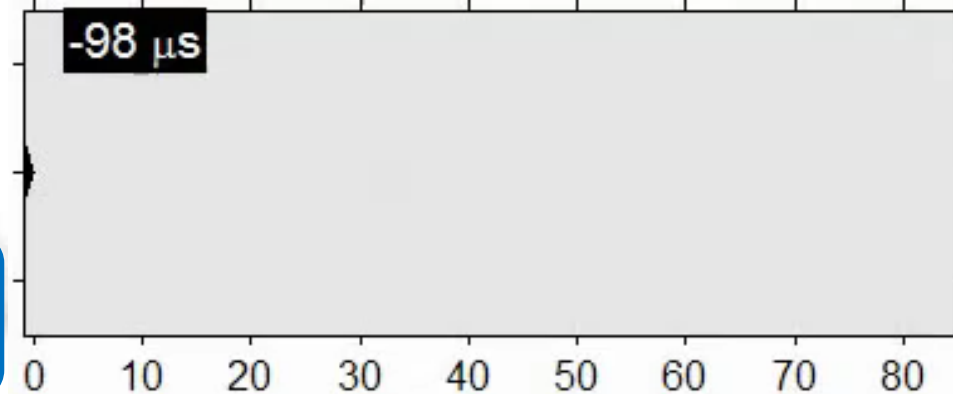
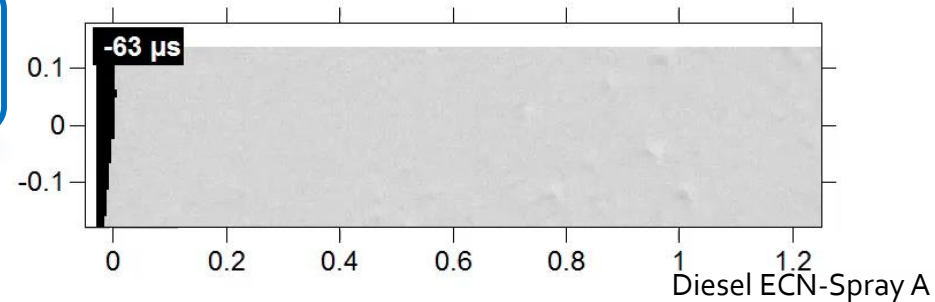
	SPRAY	COMBUSTION	TURBULENCE
CONVENTIONAL	LAGRANGIAN (DDM)	SIMPLIFIED KINETICS + TCI	RANS
ADVANCED	EULERIAN (+LAGRANGIAN)	DETAILED KINETICS + TCI	RANS → LES

Engine sprays comprises wide range of two-phase flow regimes:

GDI ECN-Spray G

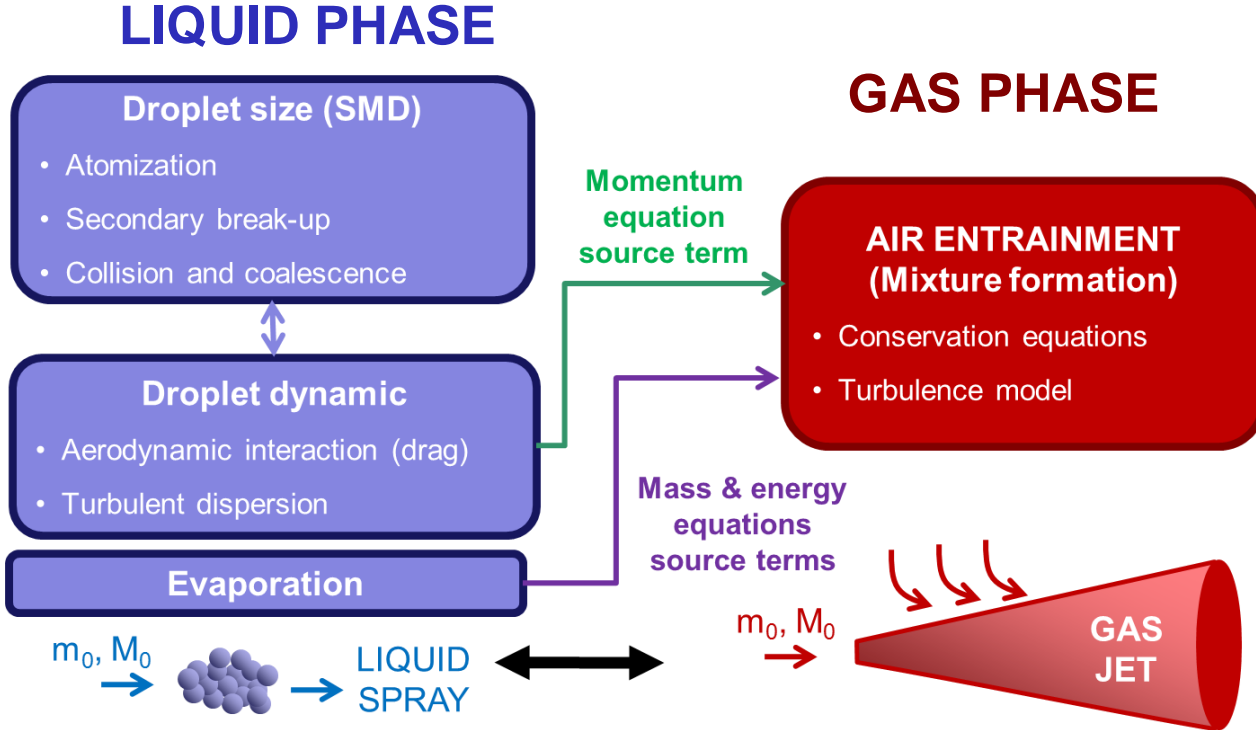
Primary Atomization /
Dense flow

Droplet Breakup /
Dispersed flow



Discrete Droplet Model:

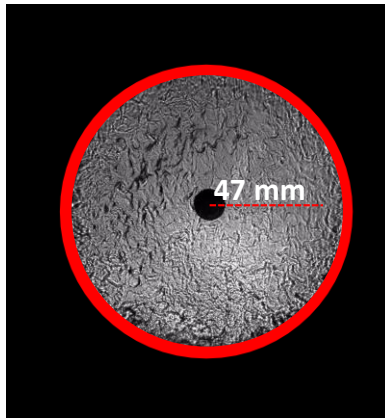
- Standard approach for engine spray CFD simulations
 - Two-fluid lagrangian liquid /eulerian gas framework
 - Phase coupling by source/sink terms between gas phase and spray eqs.



Discrete Droplet Model:

- Example of application

- *Experimental (raw image)*



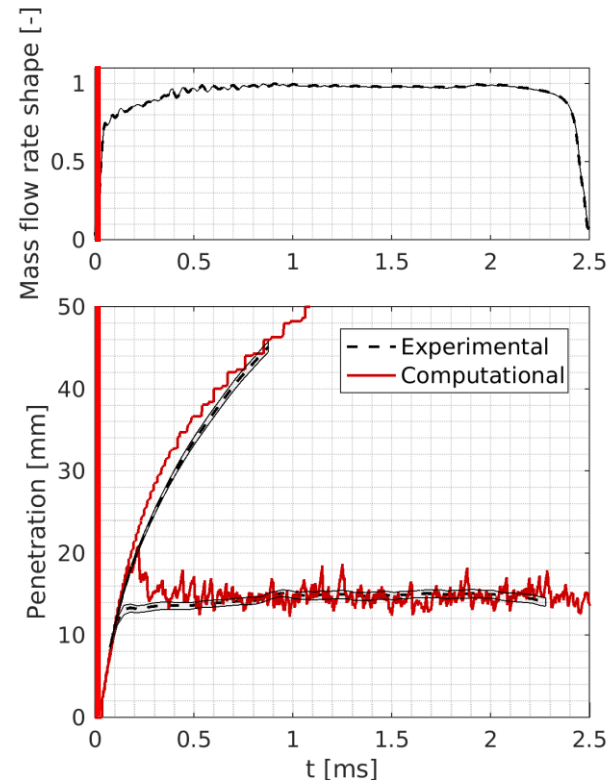
- *CFD model*



Benajes et al., FEV Diesel Powertrains 3.0 (2017)

Model calibration

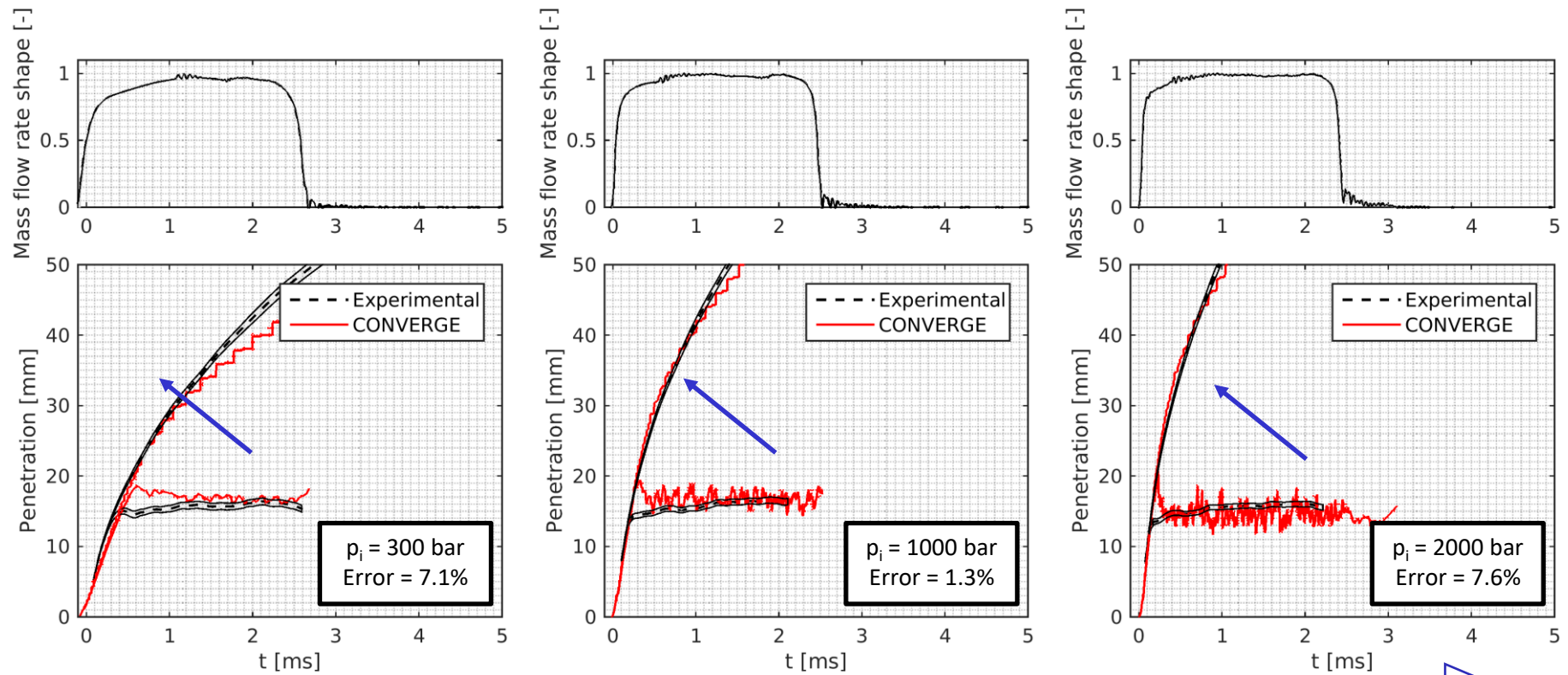
- Target: error < 5% for all testing points



Nozzle A
 T = 900 K
 $p_i = 2500$ bar
 $p_b = 50$ bar
 Error = 1.7%

Discrete Droplet Model:

- Fair accuracy after calibration using exp. data
- Example: break-up model constants (time and size) depend on P_{inj} .



Benajes et al., Diesel Powertrains 3.0 (2017)

Increasing injection pressure

$p_b = 50 \text{ bar}, T_b = 900 \text{ K}$

Discrete Droplet Model:

- Fair accuracy after calibration using exp. data
 - Example: break-up model constants (time and size) depend on P_{inj} .

Size cnst KH Time cnst KH Size cnstRT Time cnst RT

p_i [bar]	p_b [bar]	B_0	B_1	cnst3rt	rtcnst2b
300	30	0.80	5	0.5	1.0
300	50	0.80	5	0.5	
300	70	0.80	5	0.5	1.5
1000	30	1.34	11.4	0.5	1.0
1000	50	1.34	11.4	0.5	
1000	70	1.34	11.4	0.5	1.5
1800	30	2.00	18.6	0.5	1.0
1800	50	2.00	18.6	0.5	1.5
1800	70	2.00	18.6	0.5	1.0
2500	30	5.00	25	0.5	1.0
2500	50	5.00	25	0.5	1.5
2500	70	5.00	25	0.5	1.0

Increasing injection pressure

Increasing ambient pressure

KH model

$$\frac{dr_p}{dt} = -\frac{(r_p - r_c)}{\tau_{KH}}$$

$$r_c = B_0 \cdot \Lambda_{KH}$$

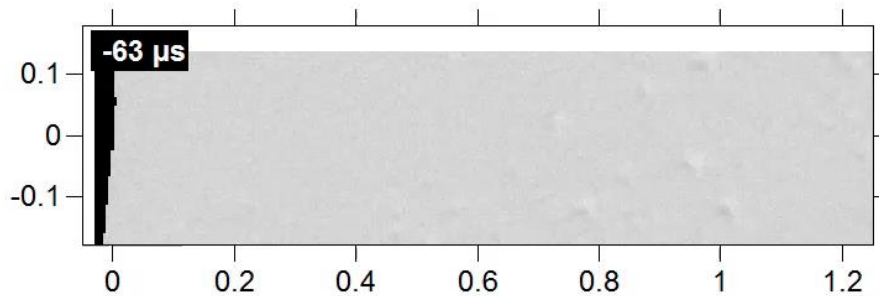
$$\tau_{KH} = \frac{3.726 \cdot B_1 \cdot r_p}{\Lambda_{KH} \cdot \Omega_{KH}}$$

Near-nozzle flow:

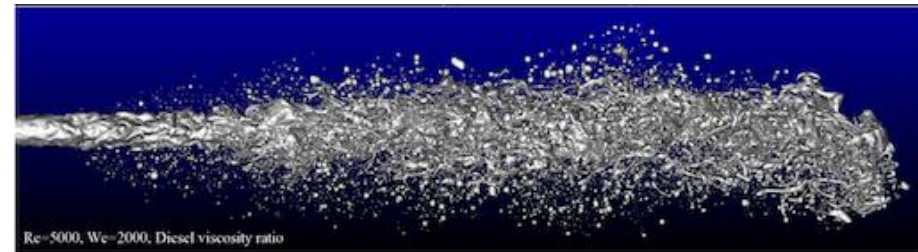
- Complex liquid-gas interface
- Modeling (*and experiments*) should move away from the droplet concept within the spray dense core
 - DDM not well suited for this region
 - ICM unfeasible ($\uparrow\uparrow Re$ & We)



Diffuse-interface eulerian methods arises as an interesting option



ECN –SprayA near-nozzle (<https://ecn.sandia.gov/>)

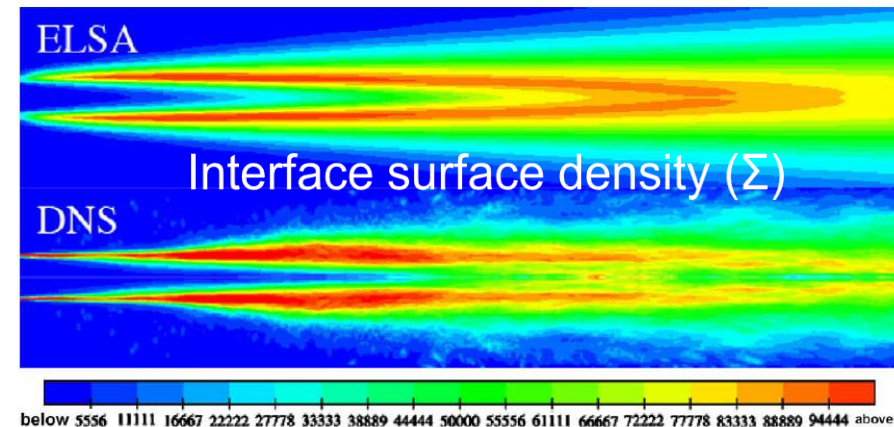
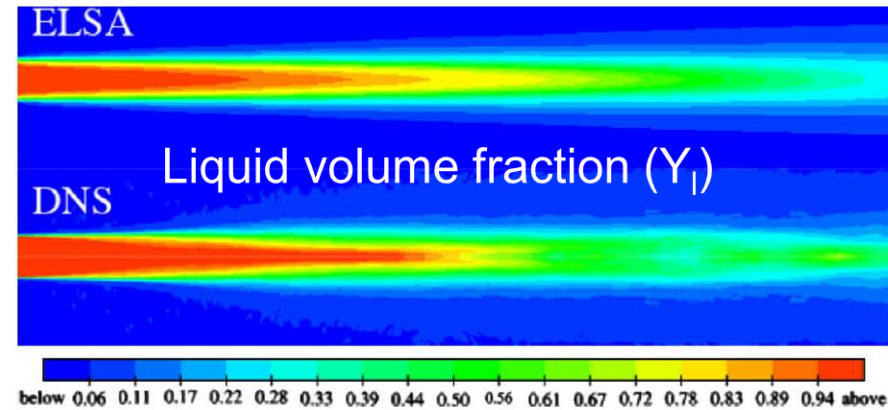


Liquid jet atomization under Diesel-like conditions, simulated on 400 million cells
<https://ctflab.mae.cornell.edu/research.html>

Eulerian diffuse-interface

approach (Vallet & Borghi, AAS (2001))

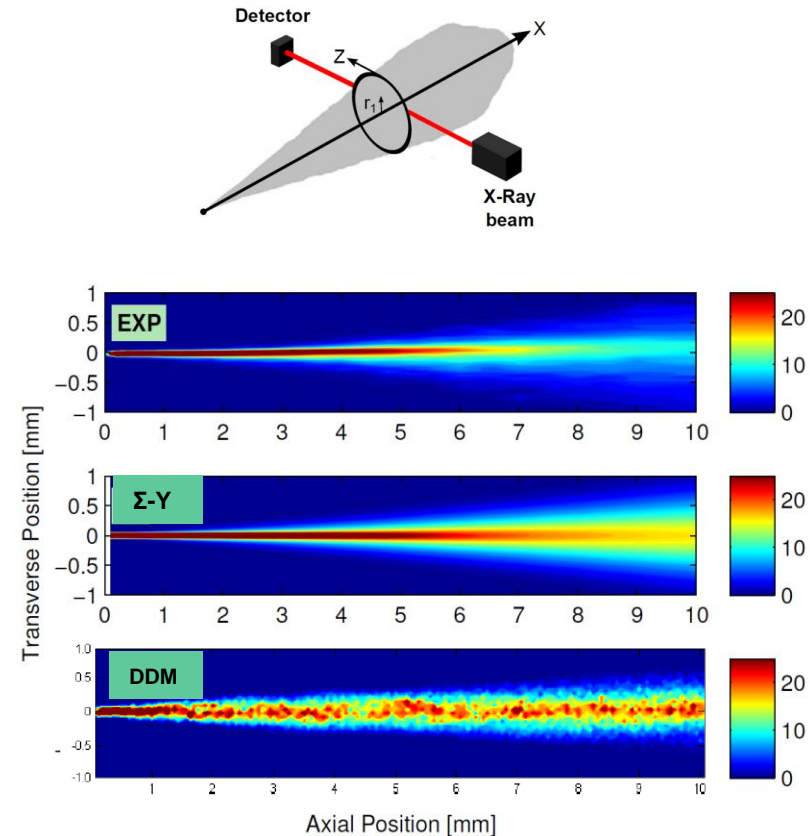
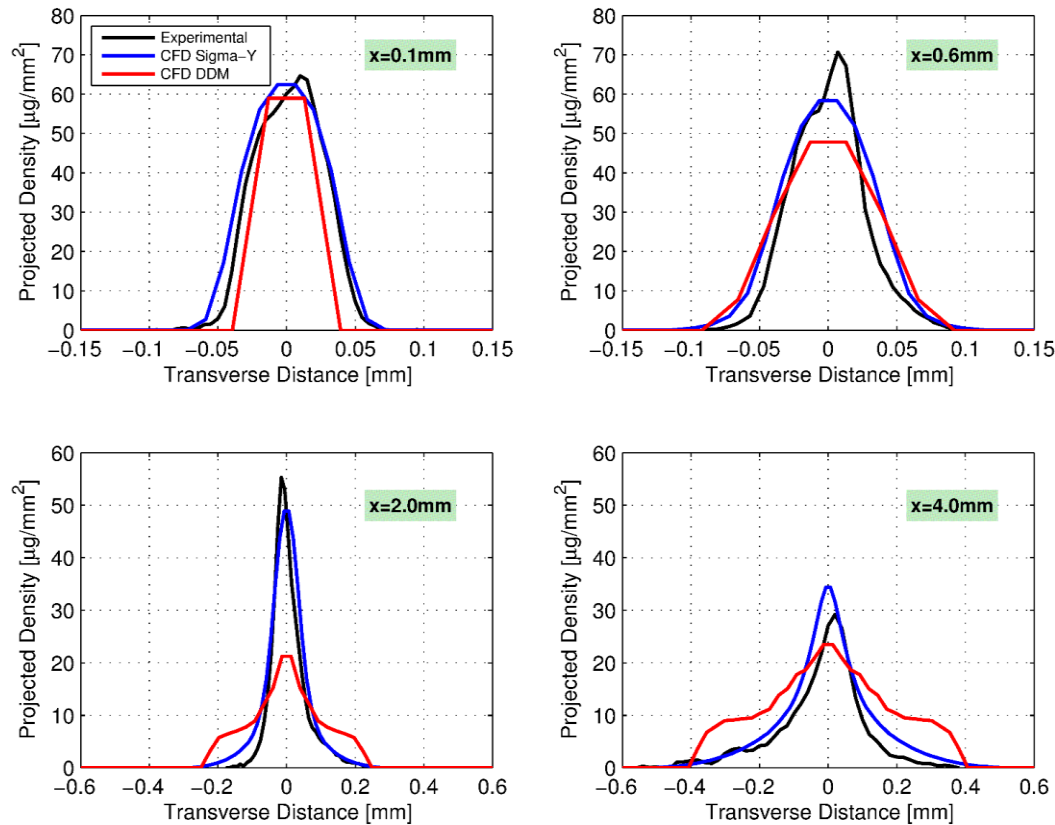
- Flow scales separation at $\uparrow\uparrow Re$ & We
 - Liquid dispersion independent from atomization processes occurring at smaller scales
- Mean velocity field
 - Liquid/gas mixture considered as a single velocity pseudo-fluid
- Liquid mass dispersion
 - Modeled as turbulent mixing of variable density fluid by means of liquid mass fraction (Y) transport eq.
- Atomization process
 - Mean liquid geometry modeled by surface area of the liquid-gas interphase (Σ)



Lebas et al., IJMF (2009)

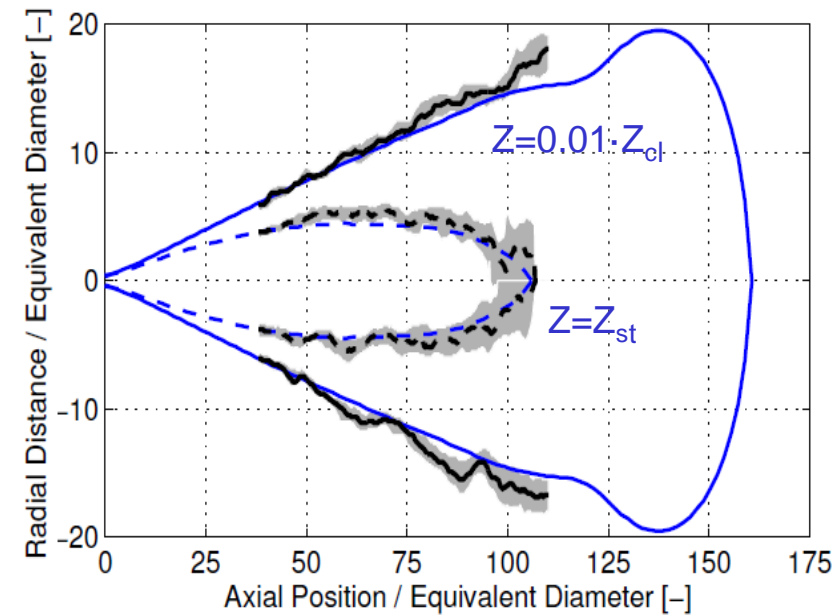
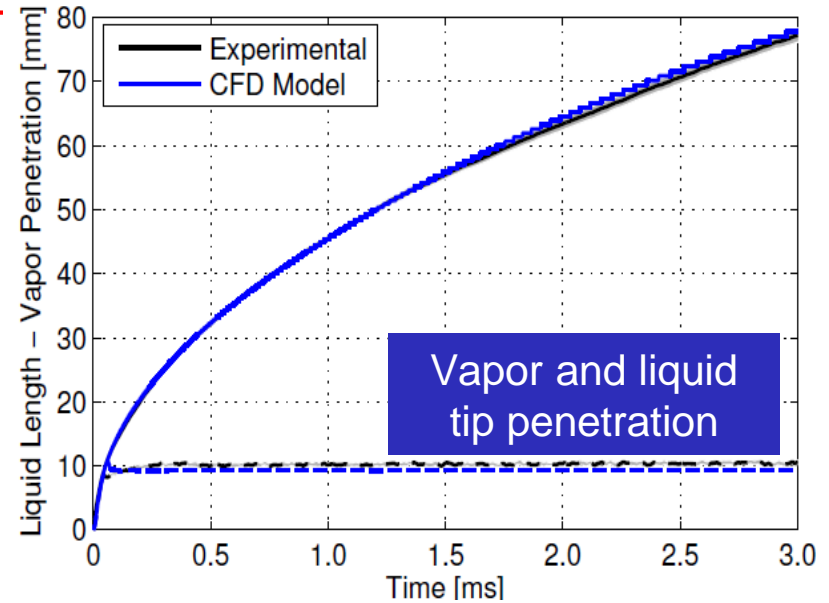
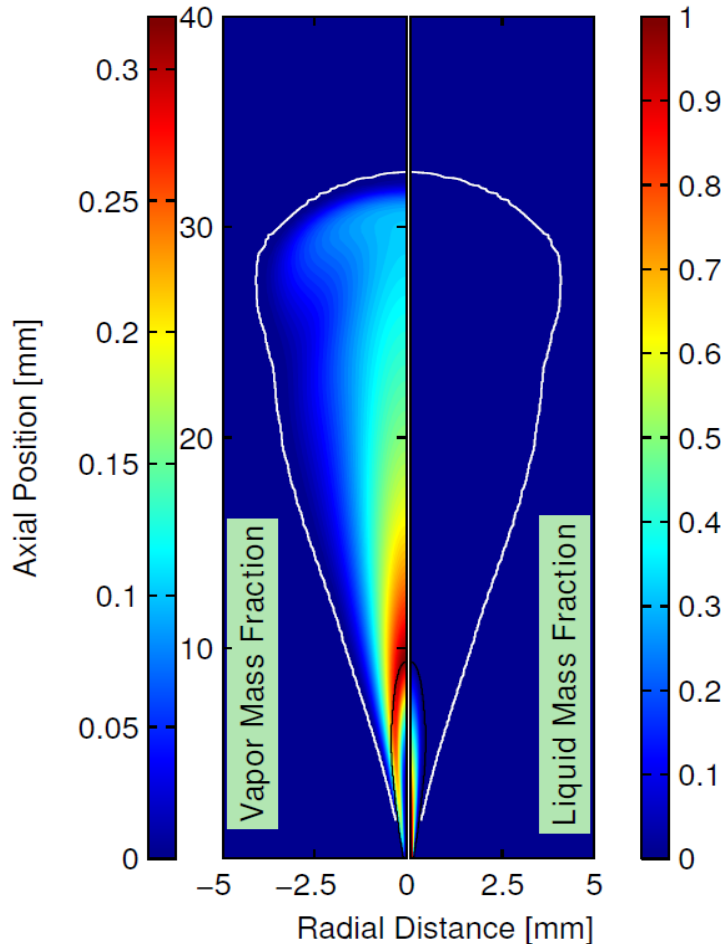
Near-field

- Improved near-nozzle liquid dispersion compared to DDM



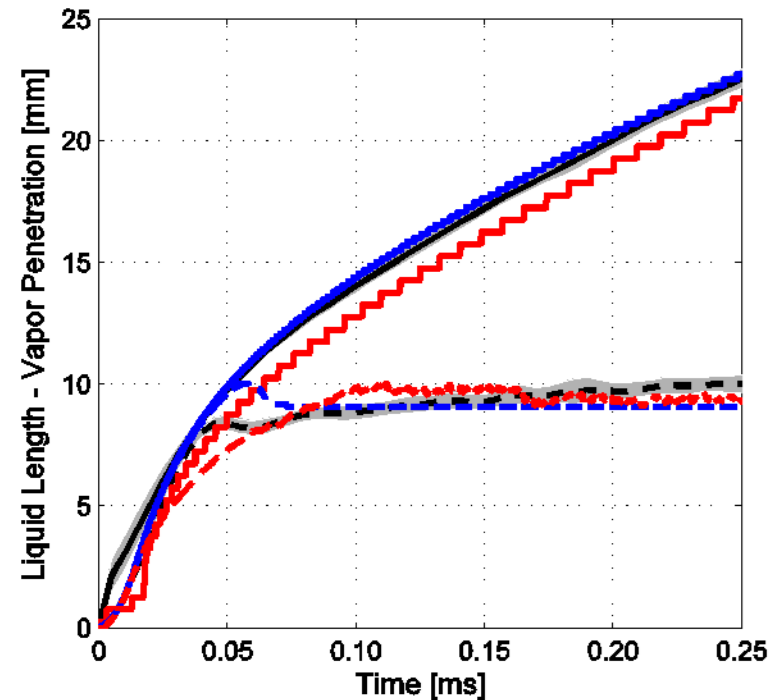
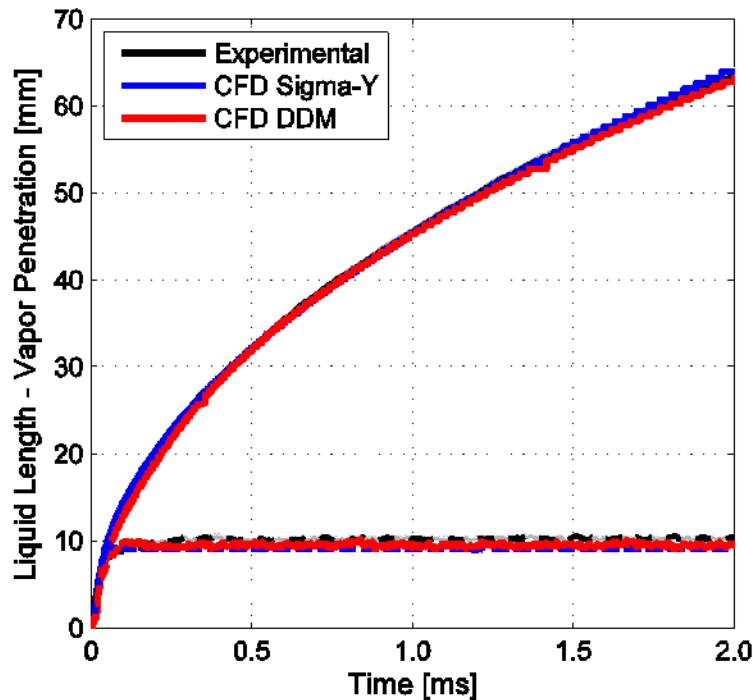
Far-field

- Consistent results downstream



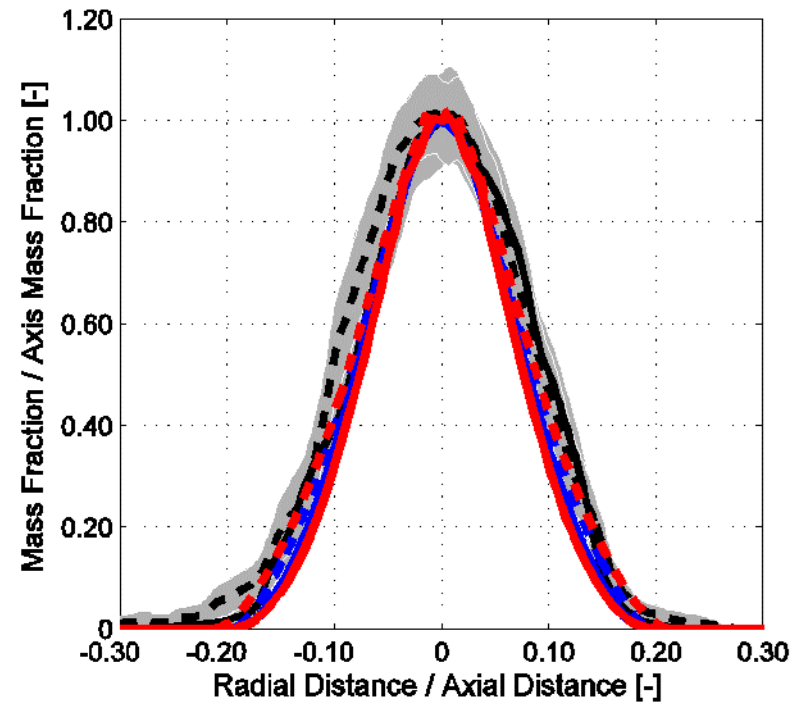
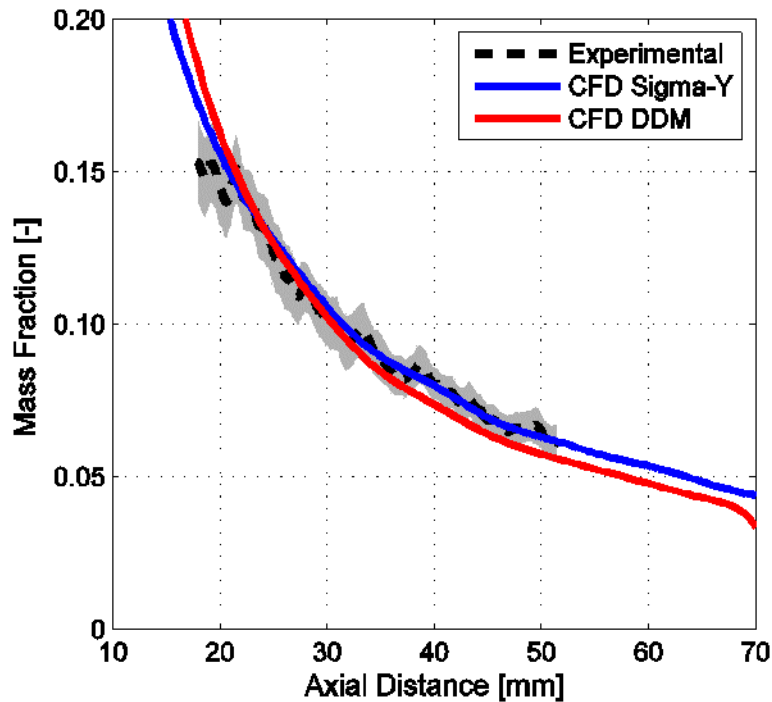
Far-field

- Improved predictions compared to calibrated DDM
 - Liquid and vapor tip penetration



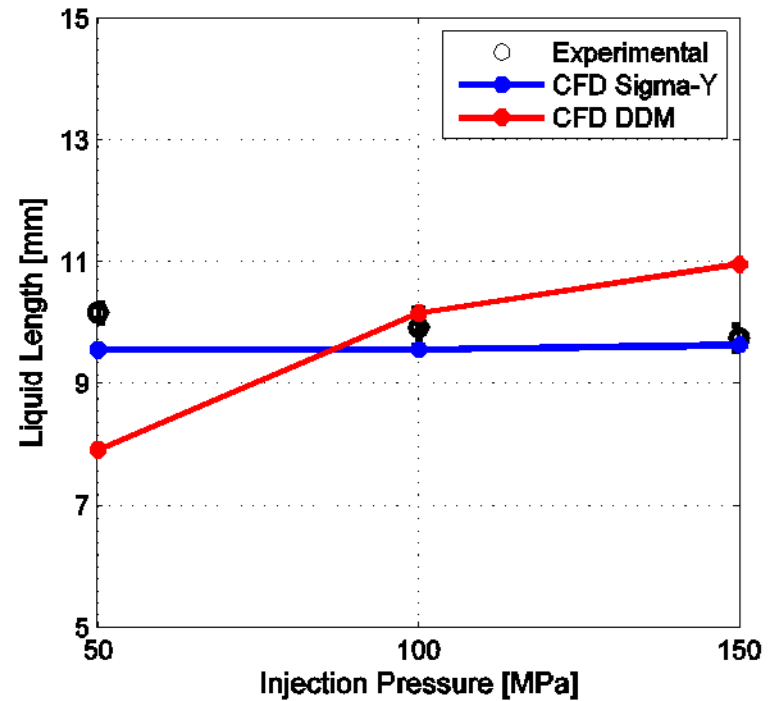
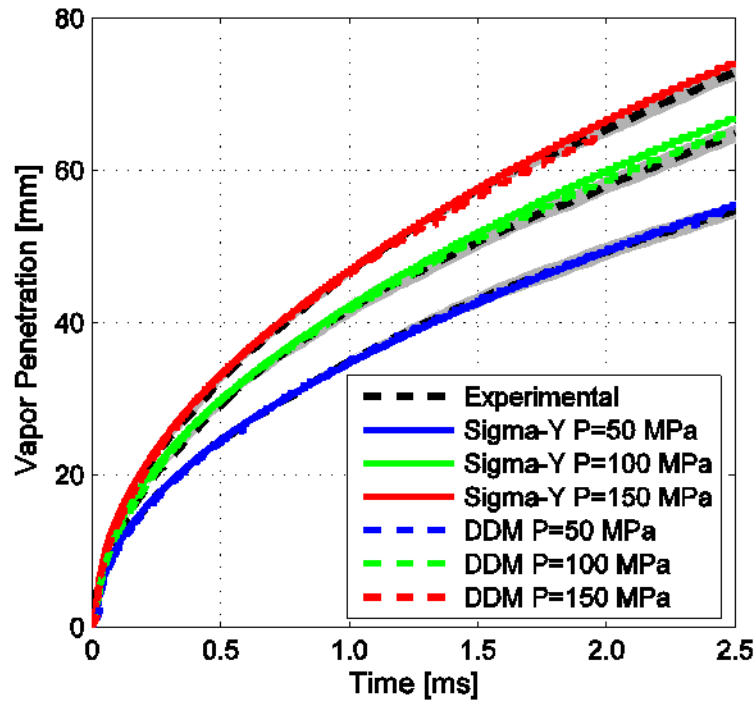
Far-field

- Improved predictions compared to calibrated DDM
 - Mixing field



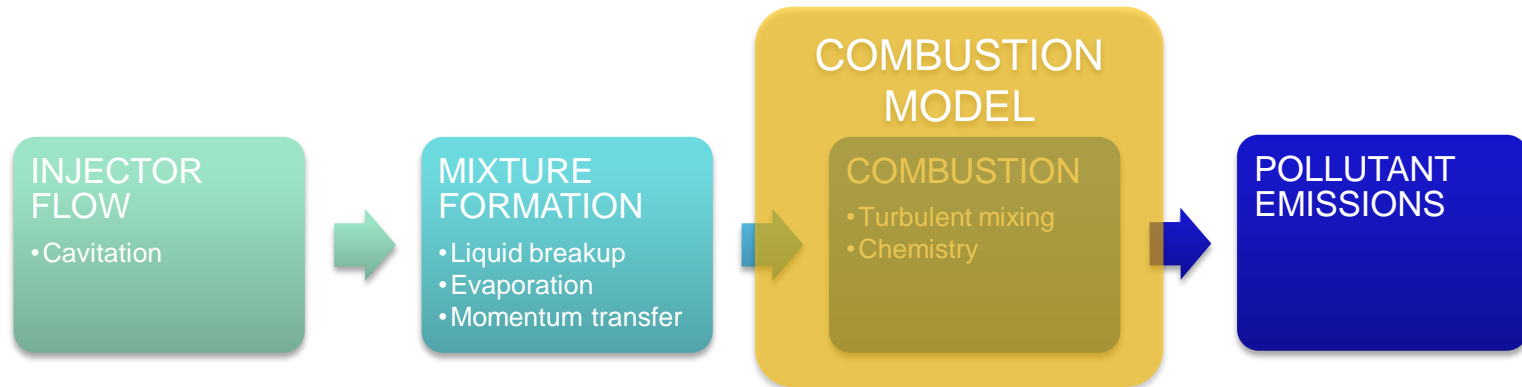
Far-field

- Proper trends on parametric variations w/o additional calibration, unlike DDM



CFD of multiphase reacting flows

- State-of-the-art and research directions



	SPRAY	COMBUSTION	TURBULENCE
CONVENTIONAL	LAGRANGIAN (DDM)	SIMPLIFIED KINETICS + TCI	RANS
ADVANCED	EULERIAN (+LAGRANGIAN)	DETAILED KINETICS + TCI	RANS → LES

CFD of reacting flows

Turbulent combustion model

Chemical Kinetics

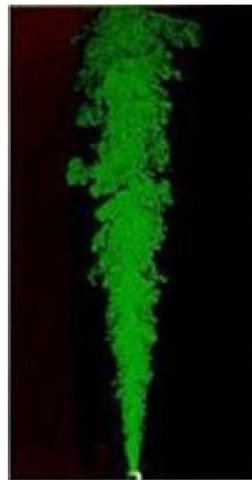
+

Turbulence
Chemistry
Interaction



CFD code

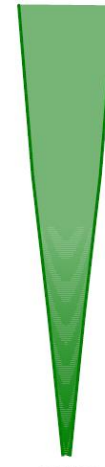
Fuel oxidation
+ Pollutant
(NOx,soot,...)



a



LES



RANS



$\tilde{w}_i?$

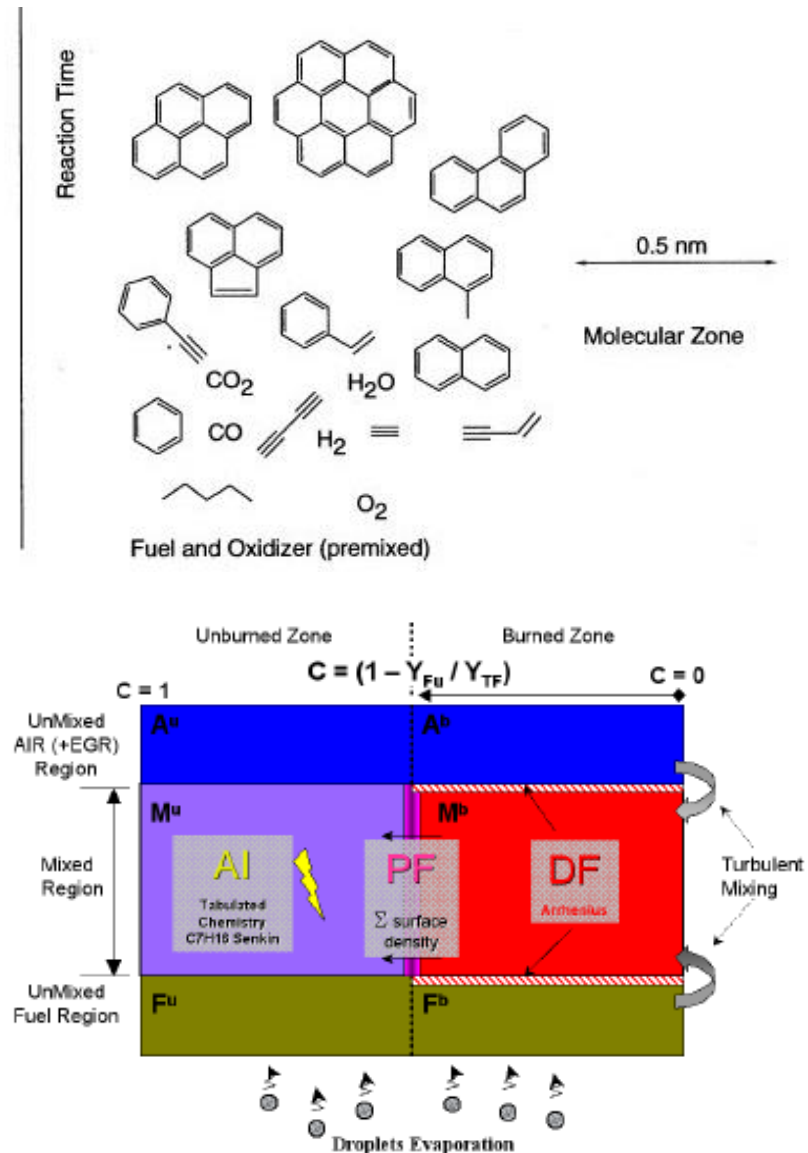
CFD of reacting flows

Chemical Kinetics

➤ From simple (1 reaction) to detailed (1000's of reactions) mechs.

TCI approaches

- Direct integration ('no model', delta-PDF,...)
- Phenomenological (CTC, PaSR, ECFM, ...)
- Scale separation + pPDF (RIF, UFPV, CMC,...)
- Transported PDFs,..



ECN-Spray A application

■ Set-up:

➤ *RANS*: std k- ϵ + $C_{1\epsilon}=1.55$

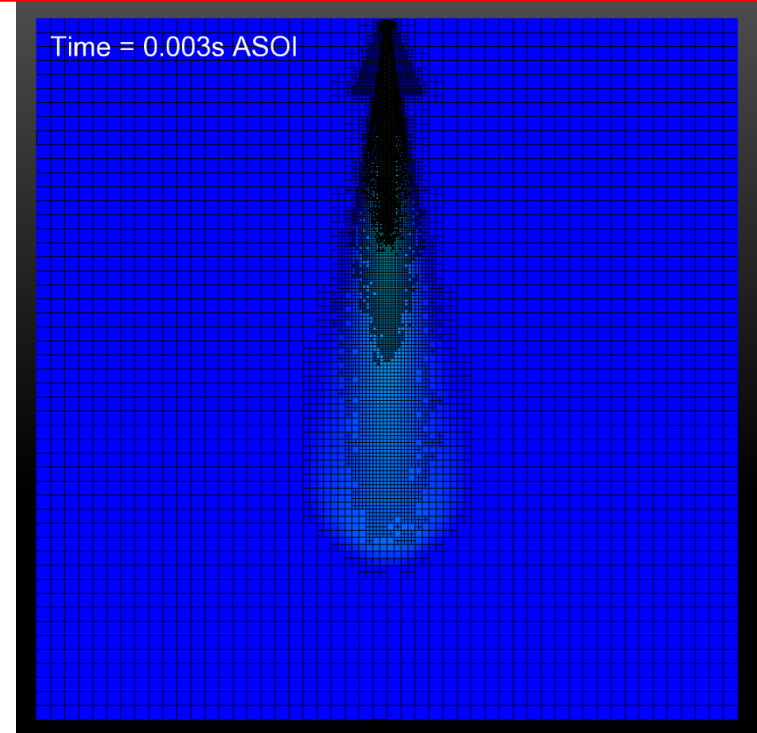
- ~1 Mcells
- Min cell size 125 μm

➤ *LES*: dynamic Structure

- ~4 Mcells
- Min cell size 62.5 μm

■ DDM spray:

➤ KH + RT atomization & break-up



■ Chemical mechs. (n-C₁₂H₂₆)

➤ Yao et al, Fuel, 2017

- 54 species / 269 reactions

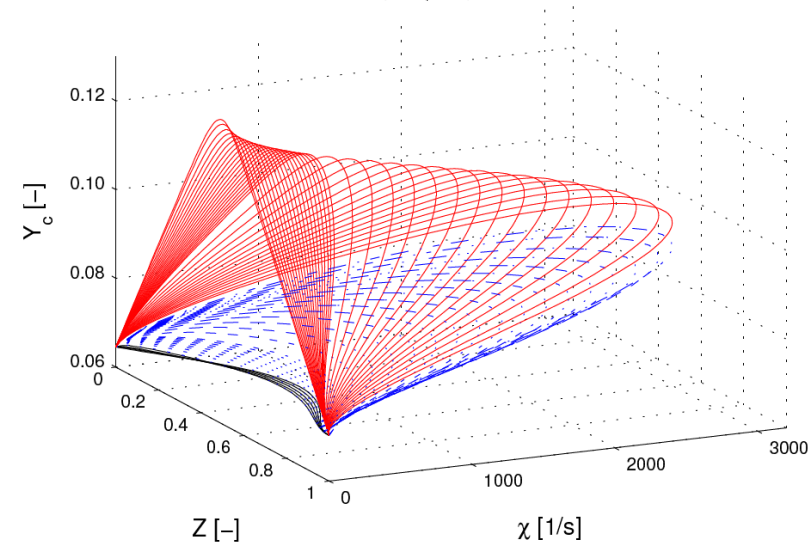
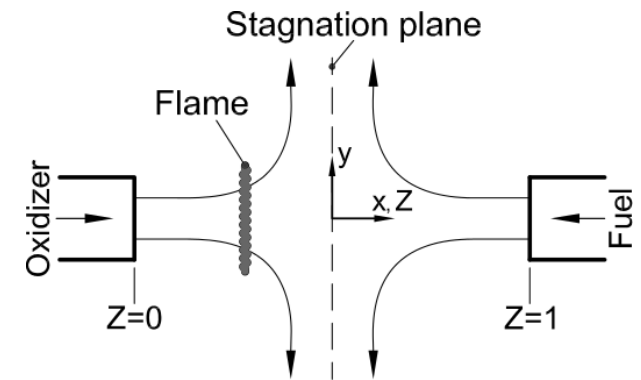
➤ Narayanaswamy et al, Comb.Flame 2014

- 255 species / 2289 reactions

TCl impact

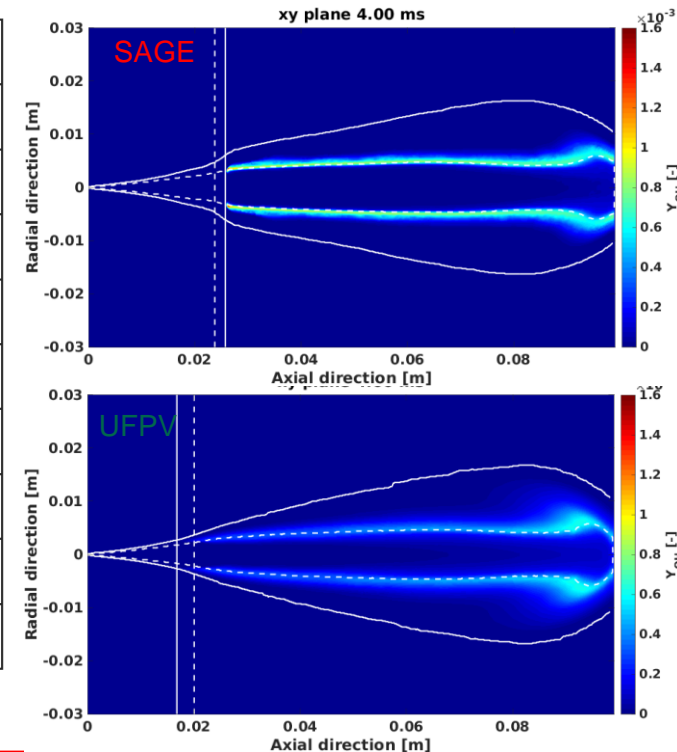
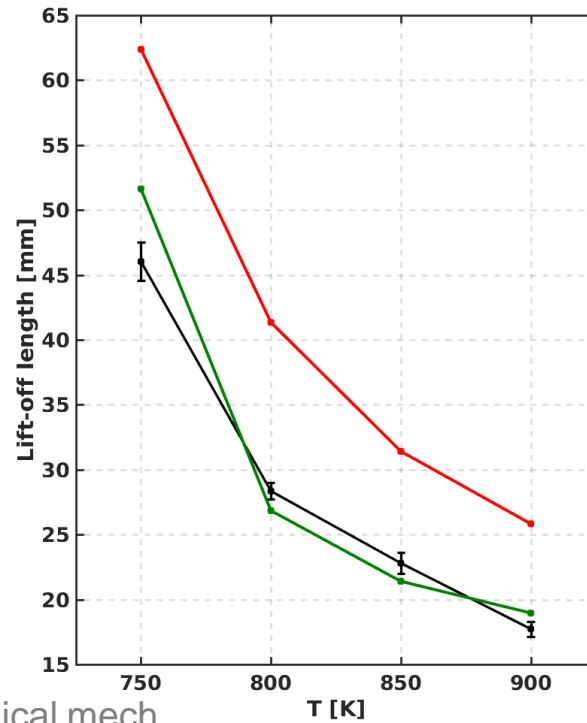
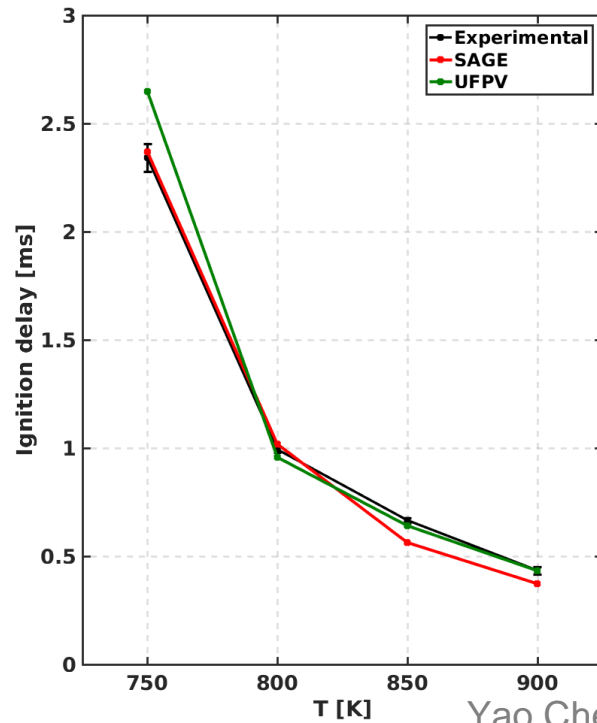
- **SAGE** (Senecal et al., 2003, SAE)
 - Detailed Chemical Kinetics Solver
 - Direct integration ('no model')

- **UFPV** (Unsteady Flamelet Progress Variable)
 - Unsteady Flamelet Model (USFM)
 - (Naud et al, CAF, 2014)
 - Tabulated chemistry → Large chemical mechanisms
 - Detailed Flamelet calculations (DF)
 - (Payri et al., AppMathModel, 2017)



TCI impact

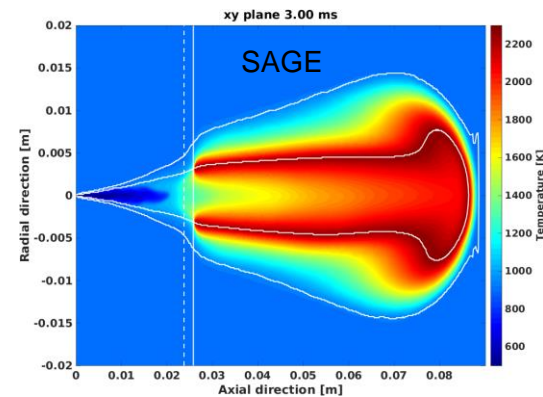
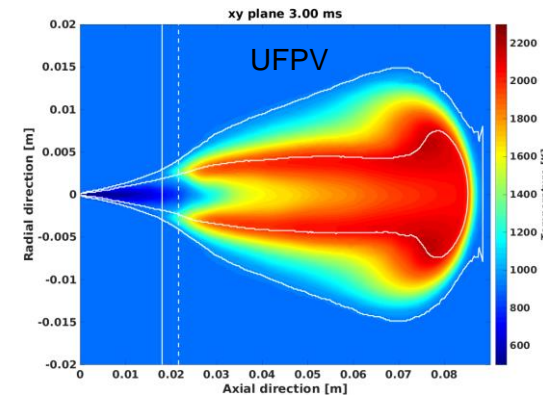
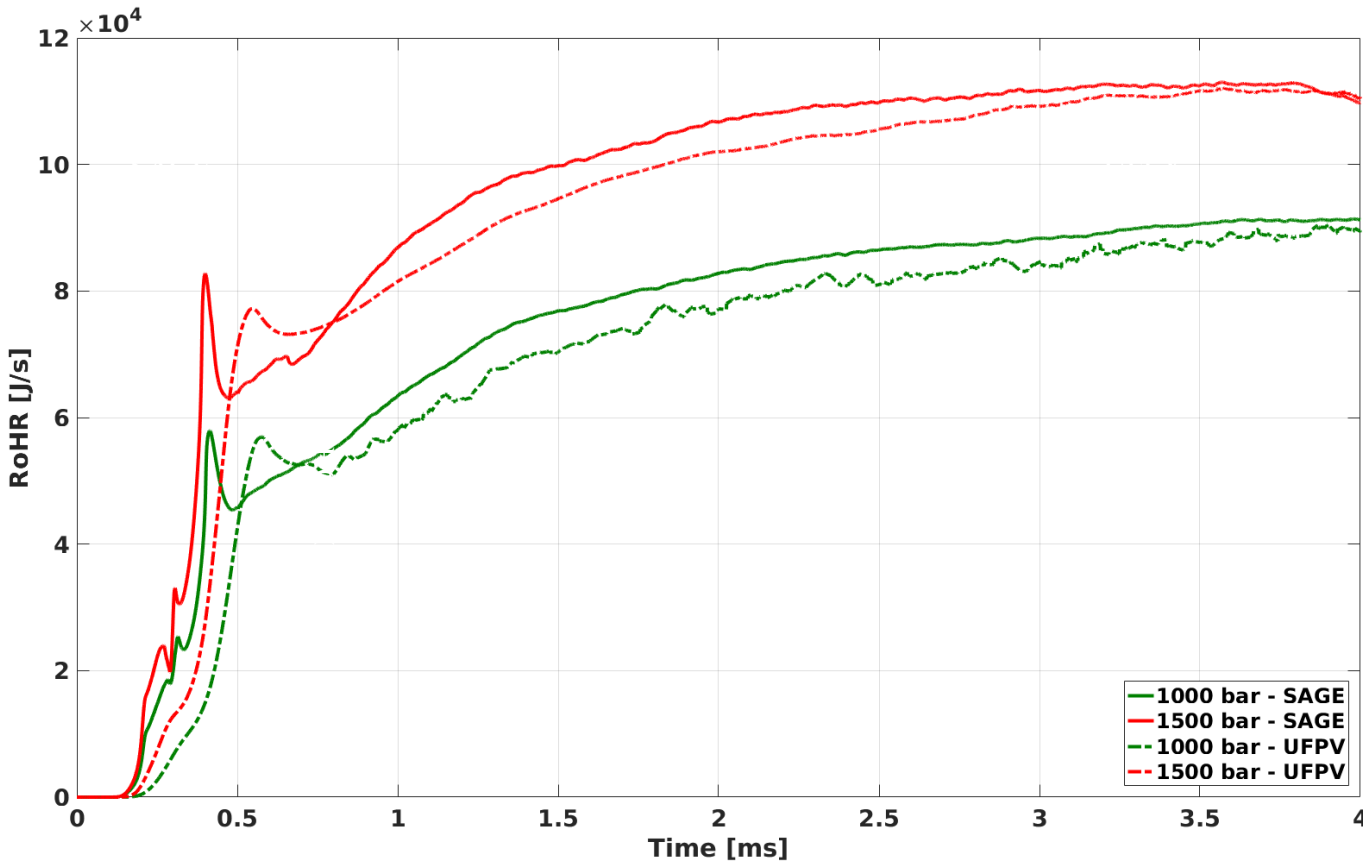
- Both models are able to capture trends
- Overall good agreement for both models in terms of ID
 - Yao mech. calibrated for reacting spray !!
- Better agreement in terms of LOL using UFPV



TCl impact

■ Heat Release

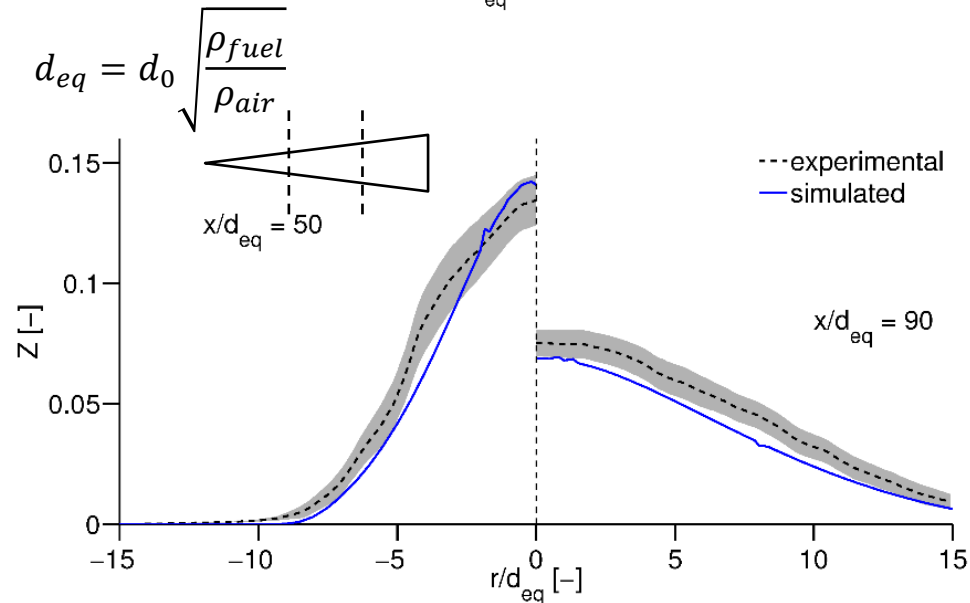
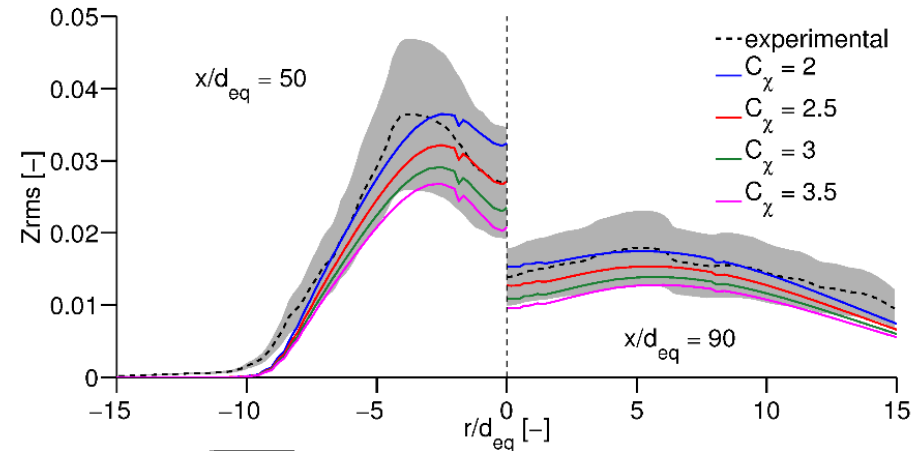
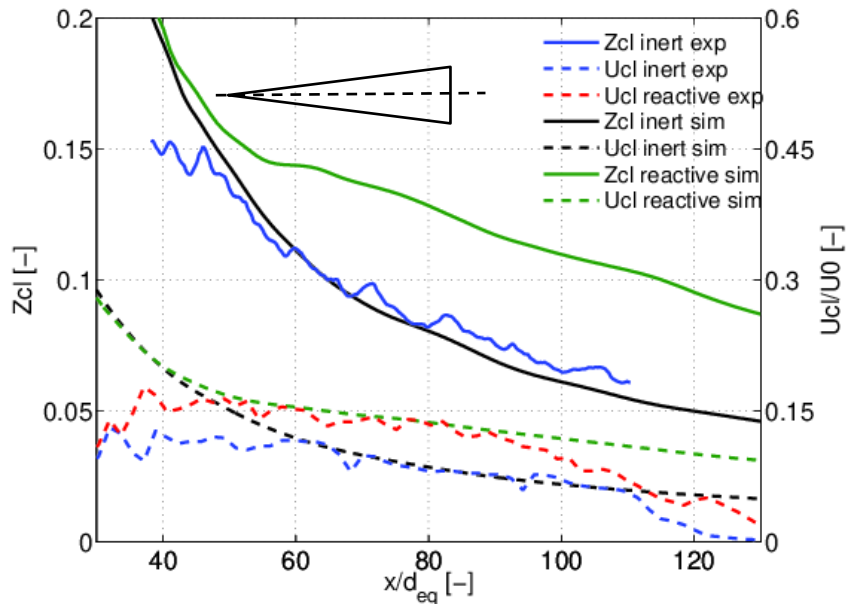
➤ Difference during premixed phase, closer during diffusion due to similar flame structure.



RANS → LES

■ Spray mixing assessment

- Fair agreement of avg. fields with RANS requires turbulence model constant adjustment

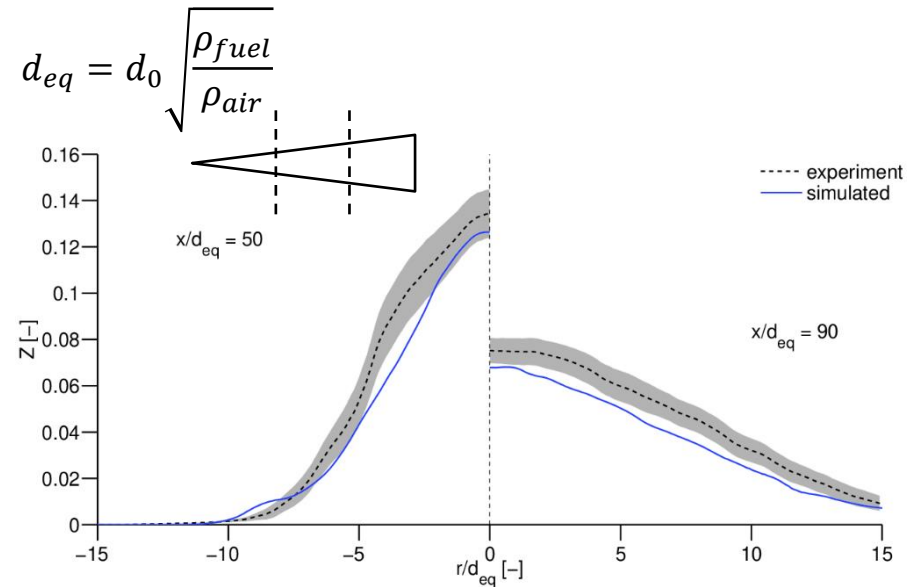
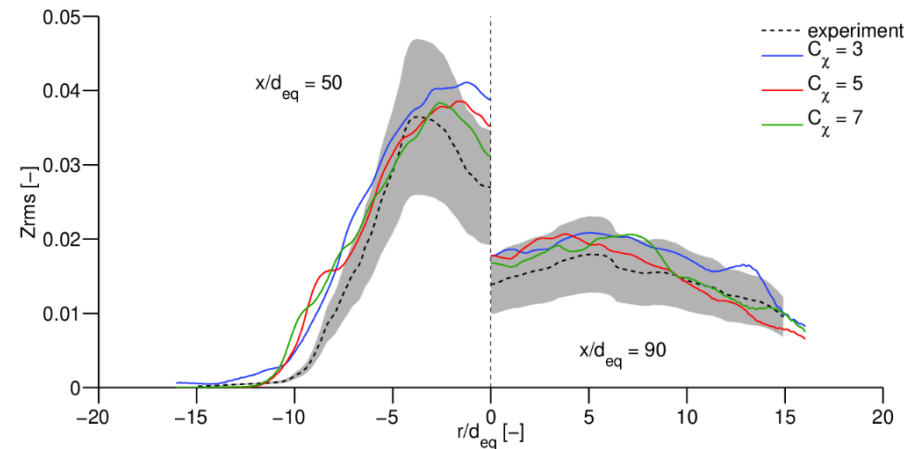
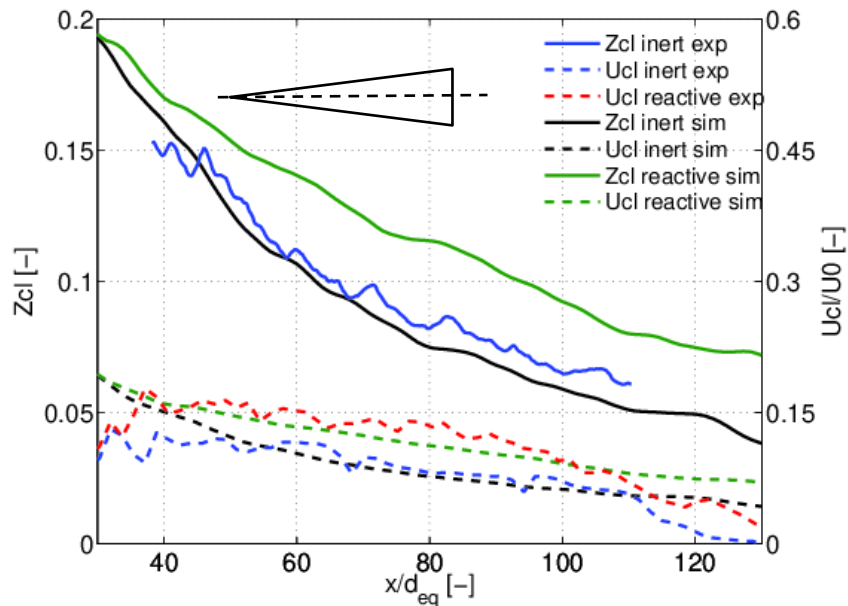


Desantes et al., Applied Thermal Engineering 117 (2017): 50–64

RANS → LES

■ Spray mixing assessment

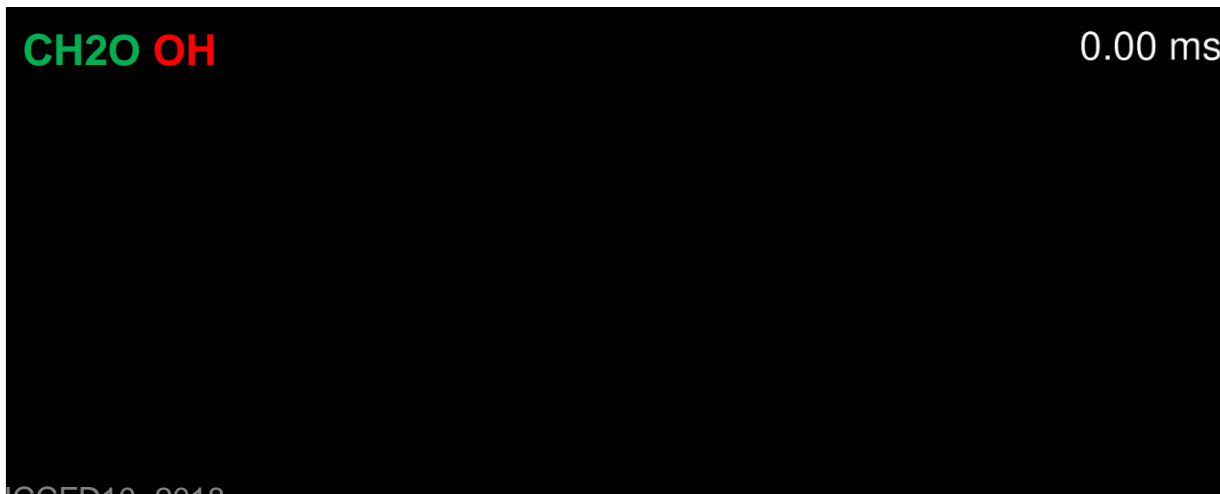
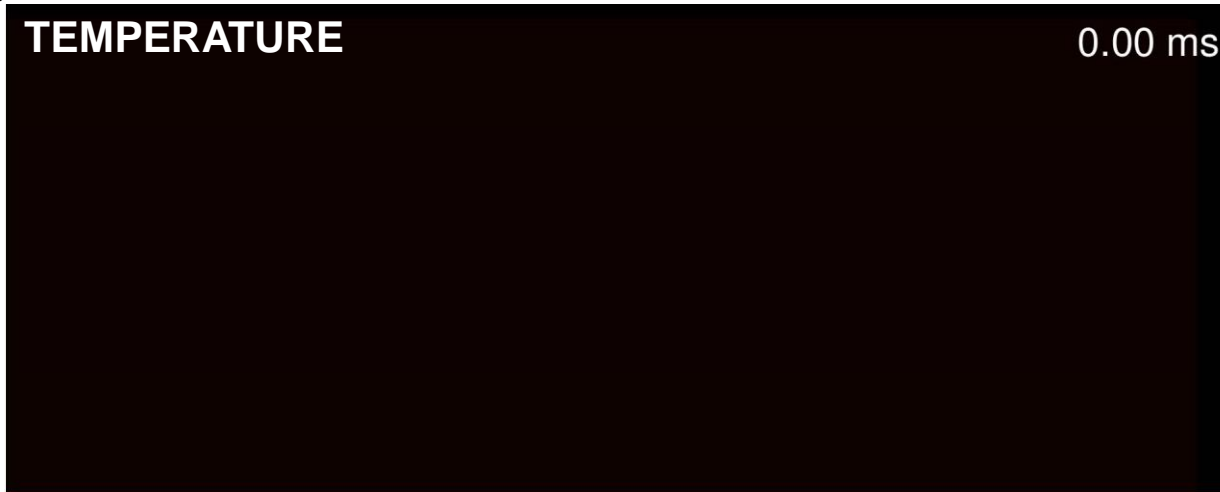
- LES provides good averaged values and lower model constant impact on fluctuations



Desantes et al., ICCFD10, 2018

RANS → LES

■ Spray flame

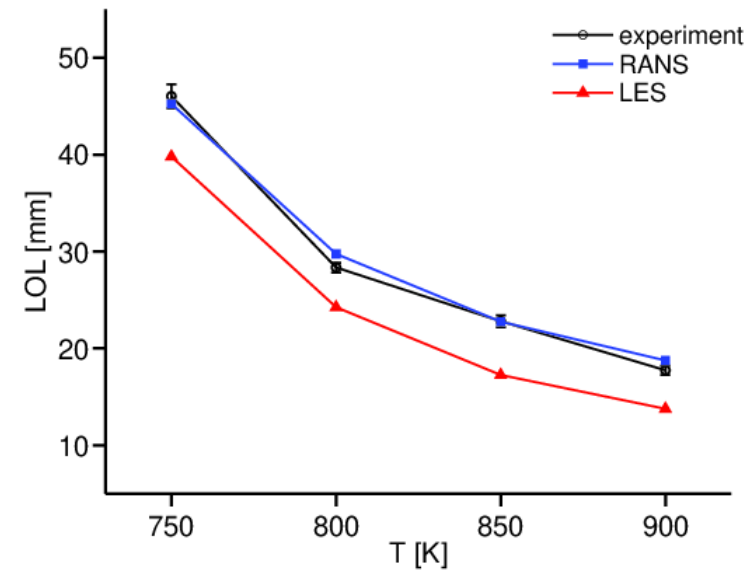
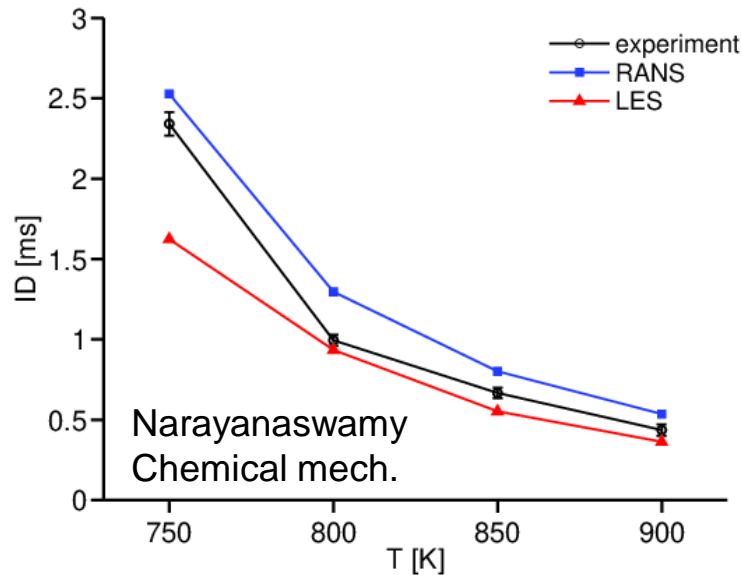


RANS → LES

■ Global combustions indicators

➤ Both ID and LOL predictions are affected by turbulence modelling approach

– Improved ID for LES using detailed mechanism, but LOL underprediction though trends are captured.

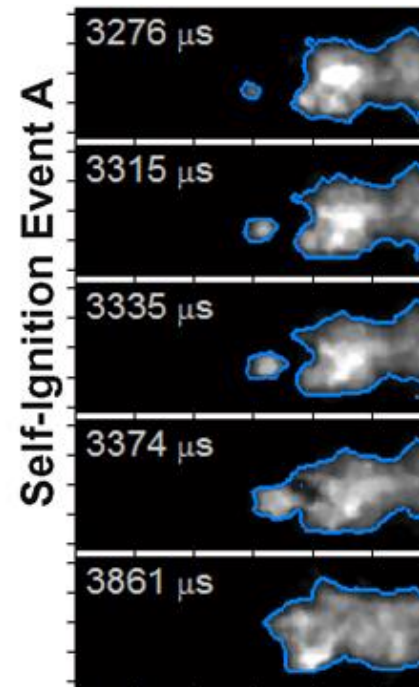
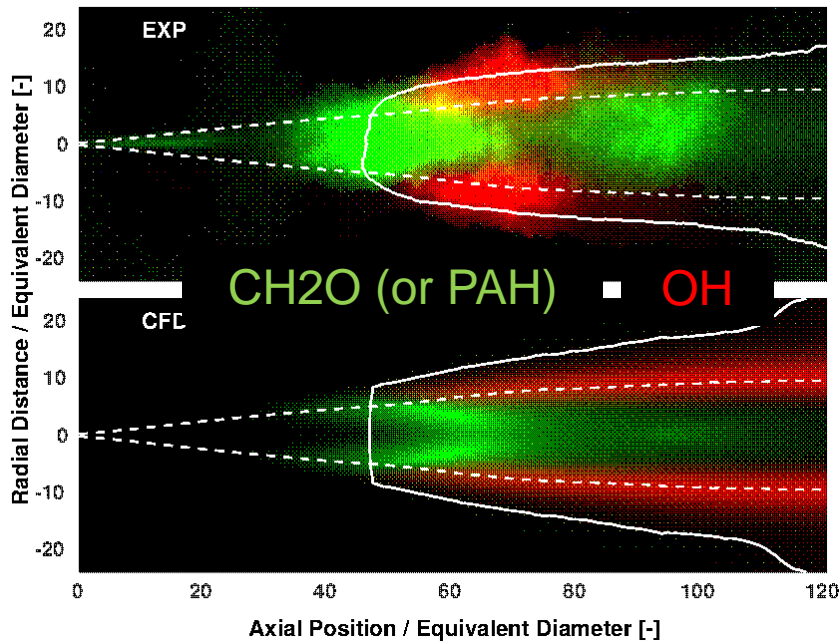


RANS → LES

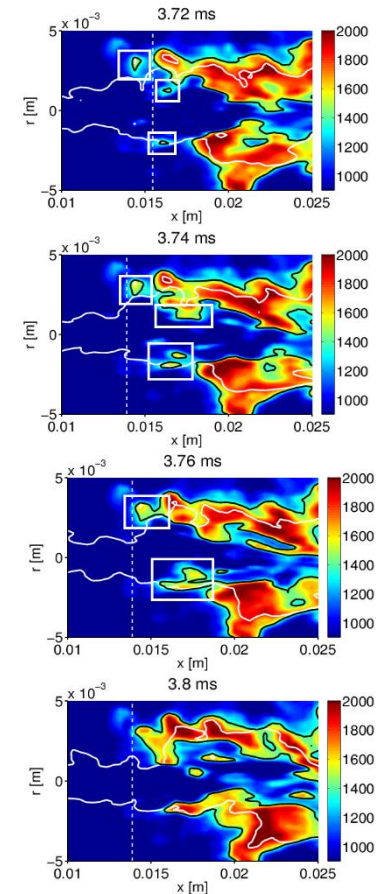
■ Flame structure

- Both RANS and LES simulations produce meaningful results

- LES is able to capture transient phenomena such as detached ignition kernels and LOL stabilization, observed in experiments.

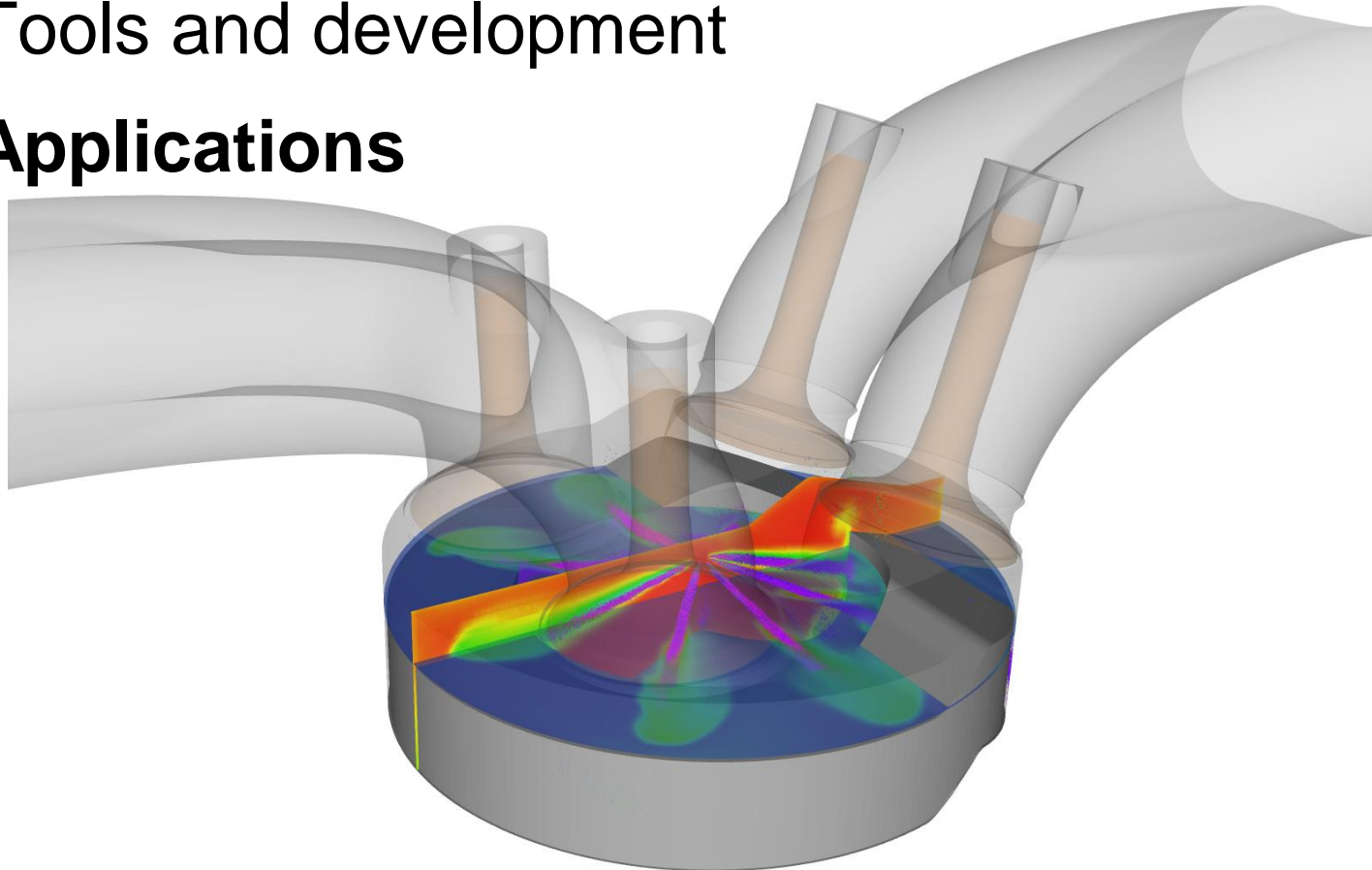


Pickett et al., PCI,32 (2009)



CONTENTS

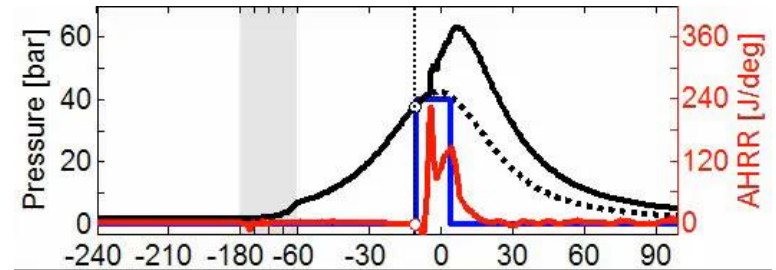
- Background and approach
- Tools and development
- **Applications**



Framework

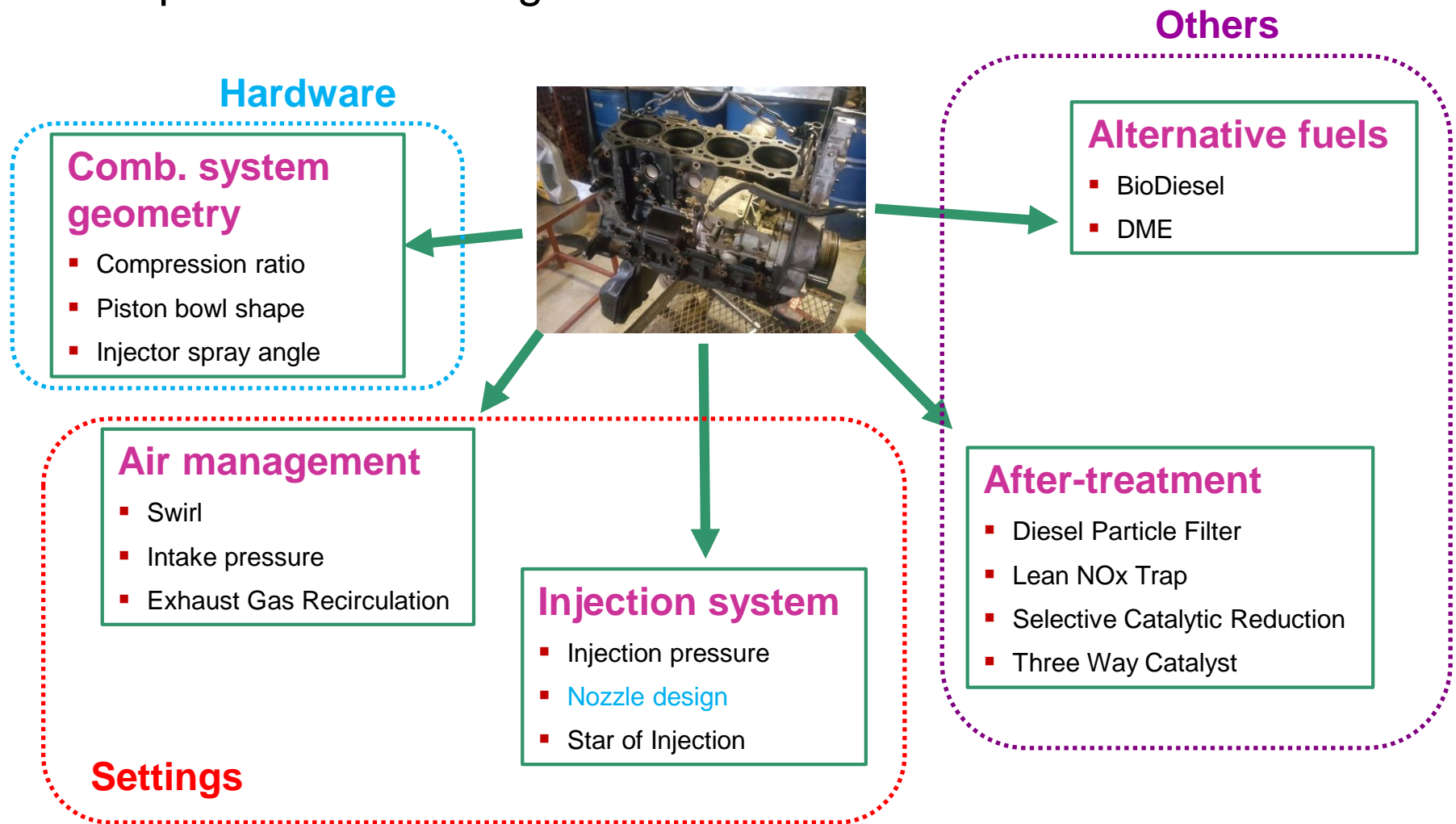
■ Convention Diesel Combustion

- Widely used due to high efficiency and reliability.
- Difficult to simultaneously reduce fuel consumption and emissions (NO_x-Soot trade-off) without complex after-treatment.
- Alternative CI strategies (PPC, HCCI, ...) still limited application due to ignition control issues.



Framework

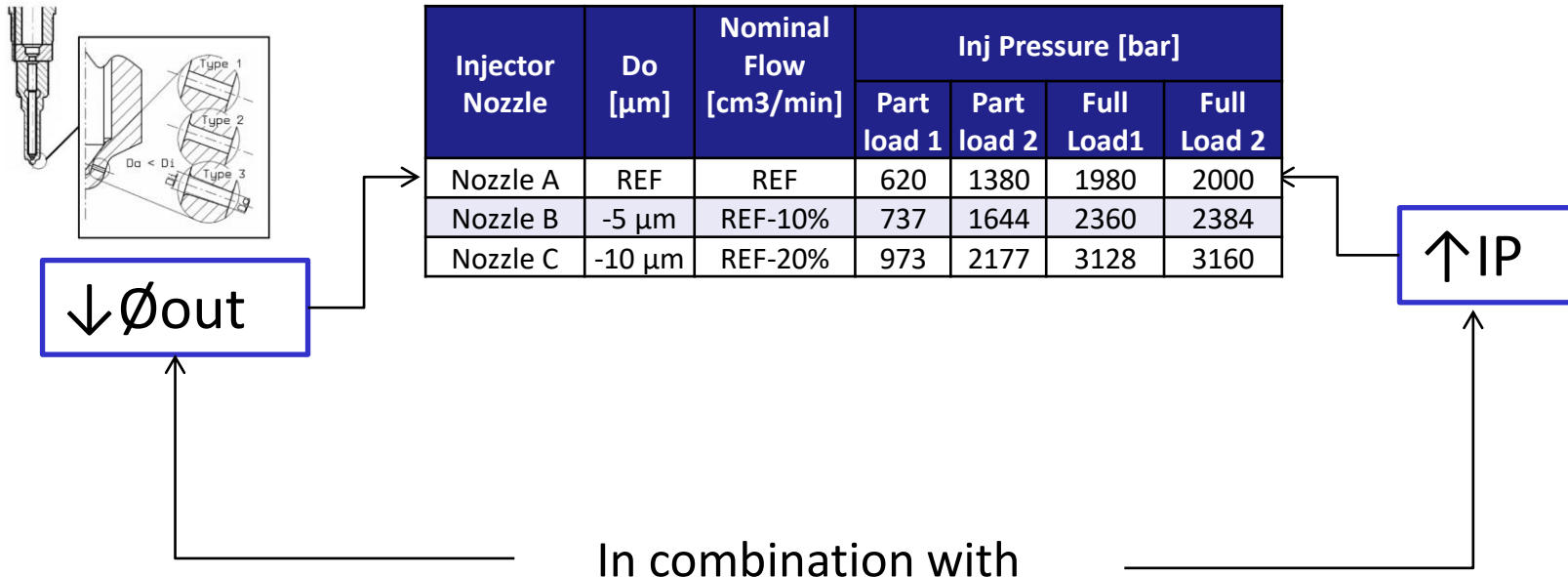
- Optimization strategies for CDC



Micro-orifice nozzles and high injection pressure

■ Objective:

- Evaluating the potential of integrating the micro-orifice nozzle technology together with a high injection pressure system for passenger car diesel engine applications



Tools & Methodology

CFD software: **CONVERGE v2.3**



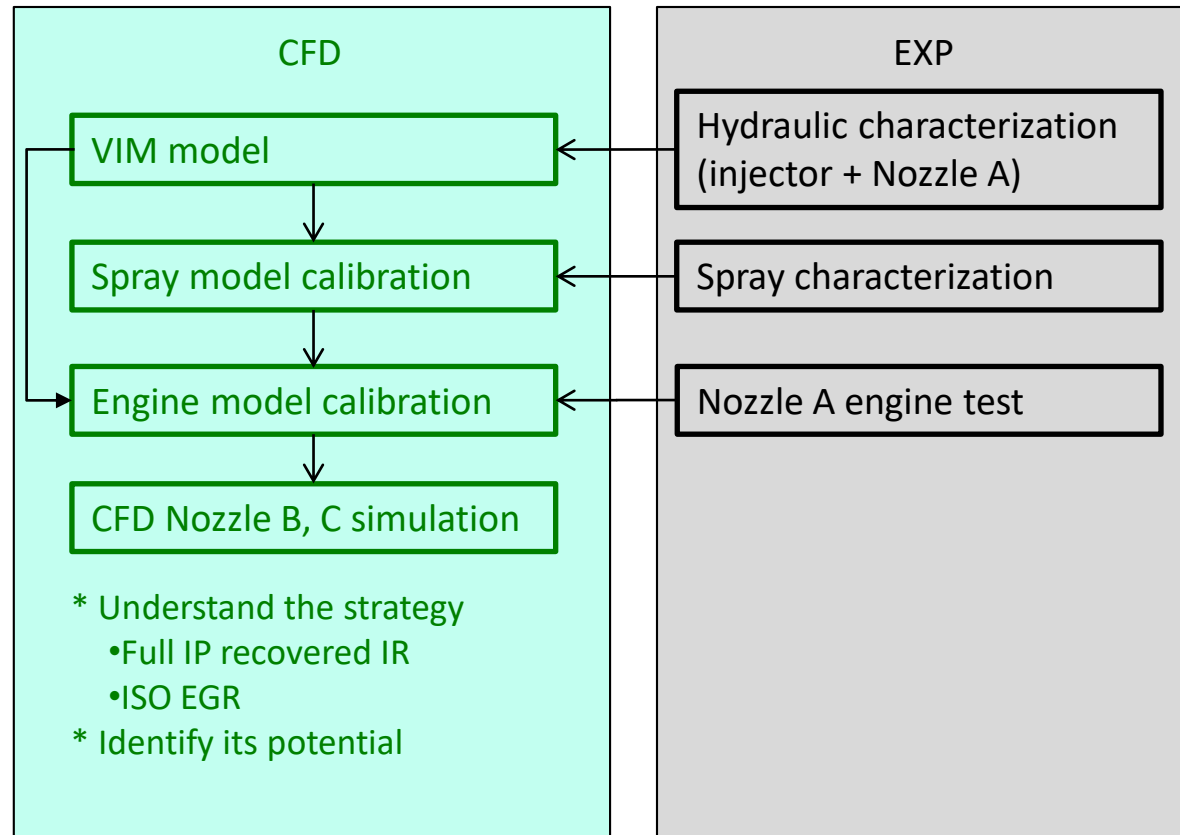
Model approach: **DDM**
 Injection model: Blob
 Atomization model: **KH-RT**

Fuel: Diesel surrogate

- N-C10H22 (71%)
- C11H22O2-MD (23%)
- A2CH3 (6%)

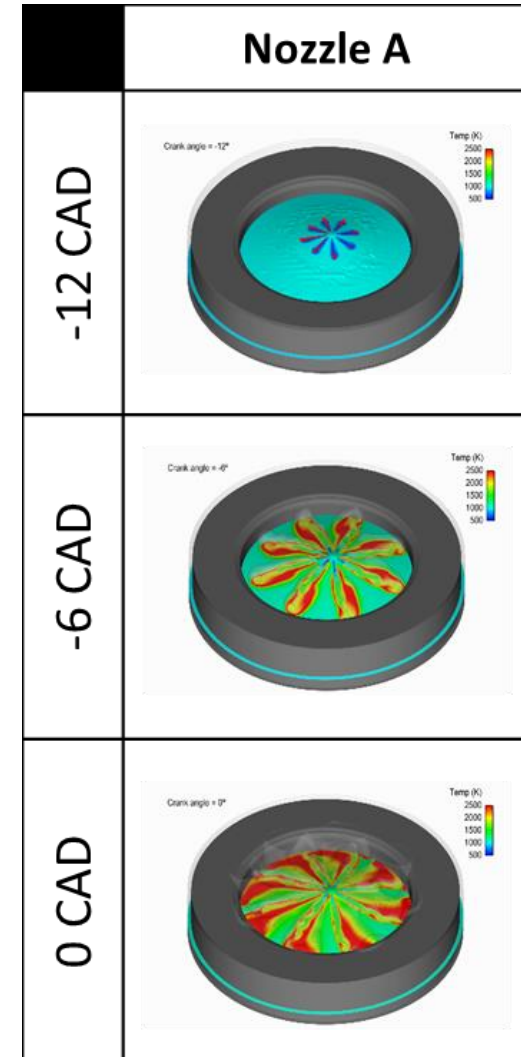
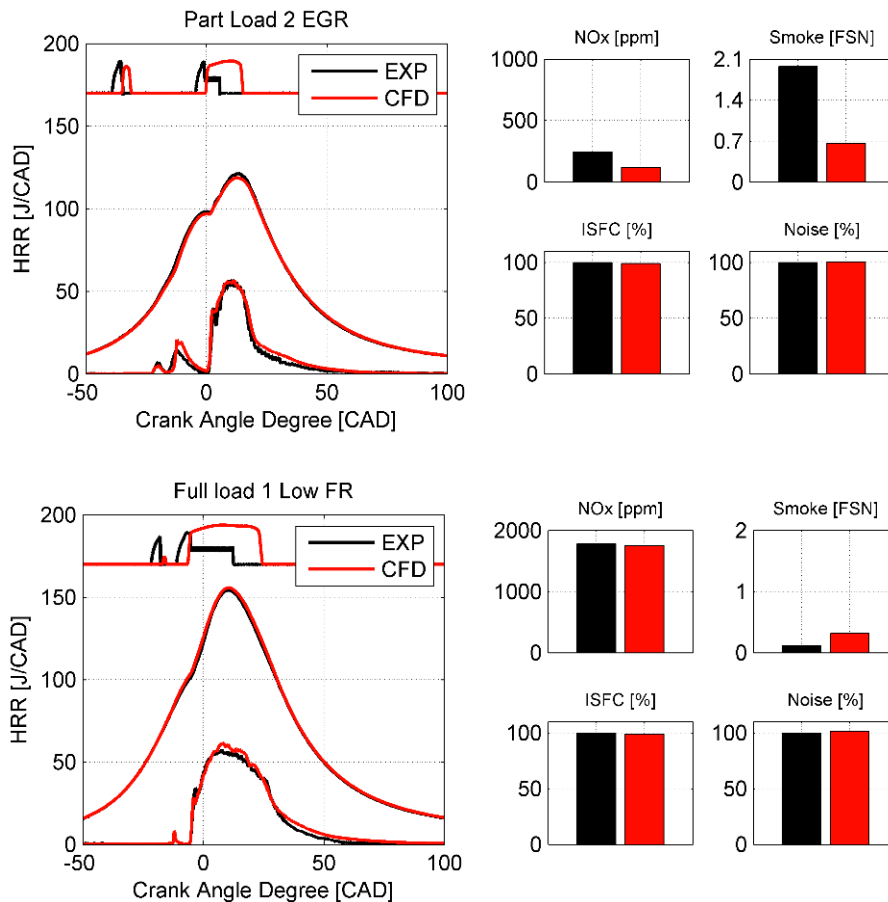
Other submodels

- Drag: dynamic drop
- Evaporation: Frosling
- Collision model: O'Rourke



Engine model calibration & assessment

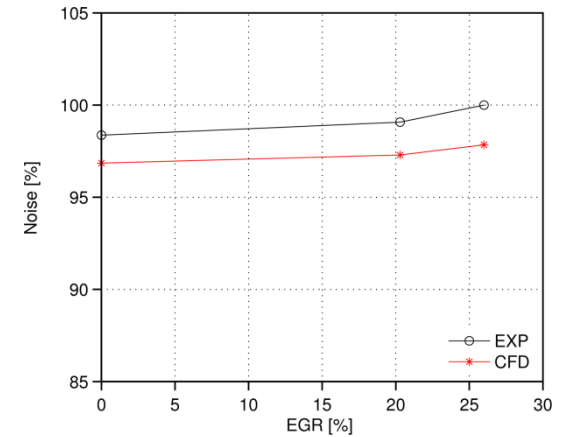
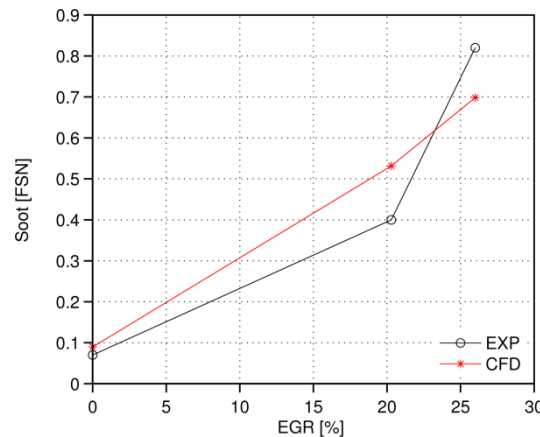
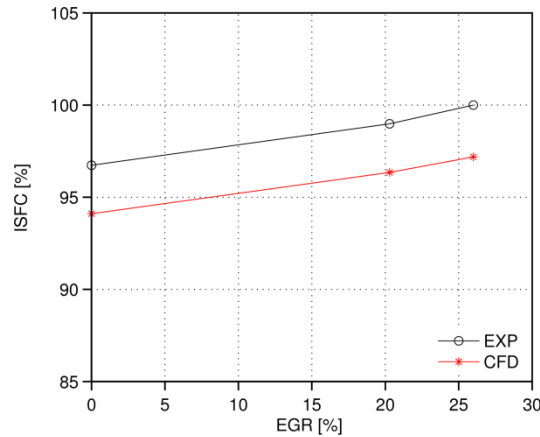
■ Part- and full-load



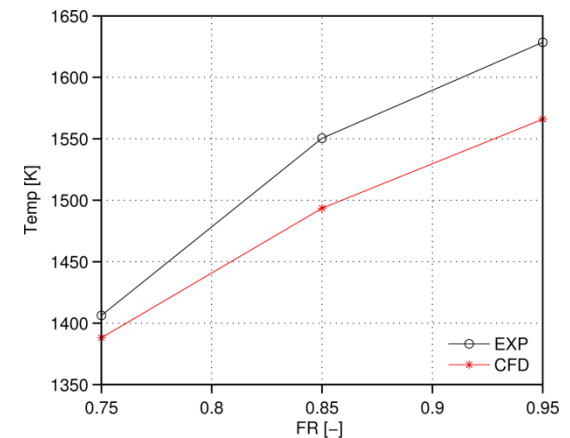
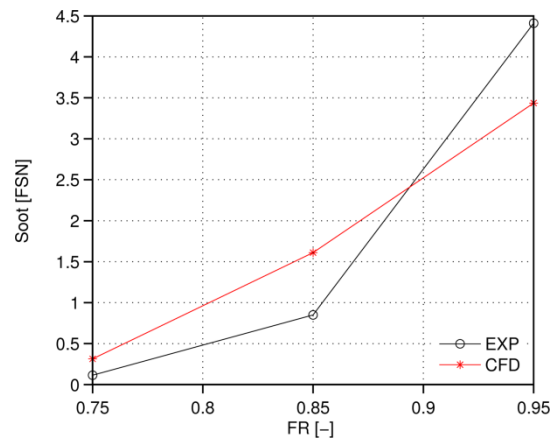
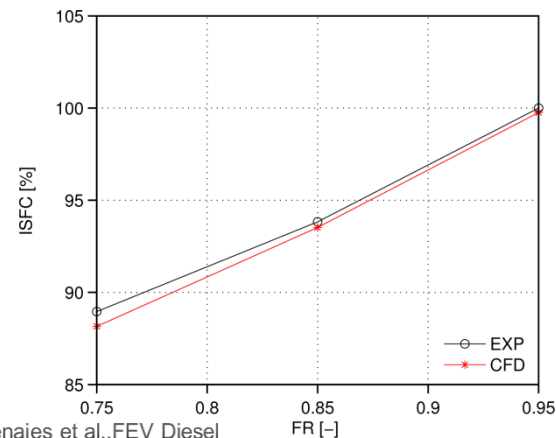
Engine model calibration & assessment

■ Part- and full-load

Part load



Full load



Benajes et al., FEV Diesel Powertrains 3.0 (2017)

Model application

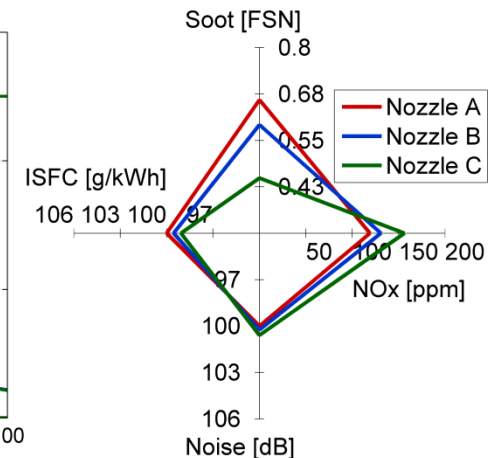
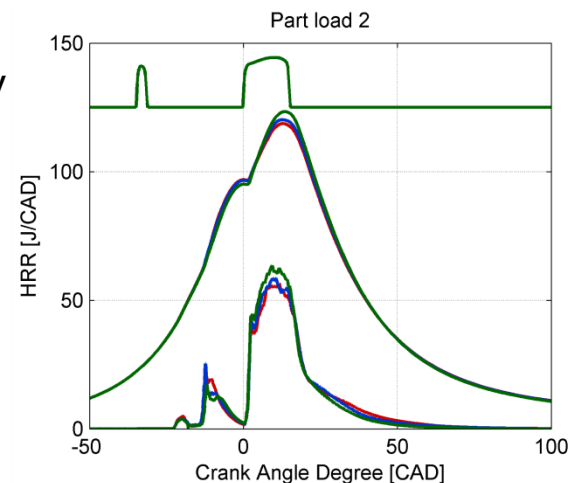
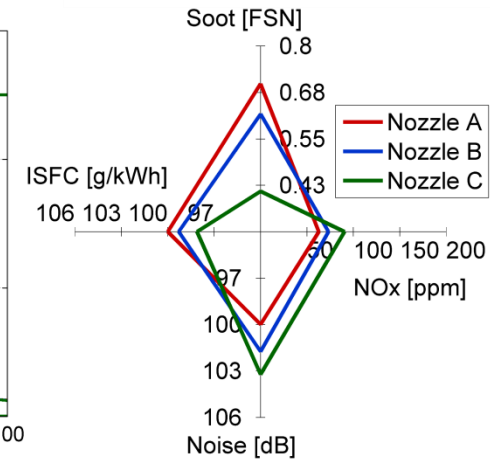
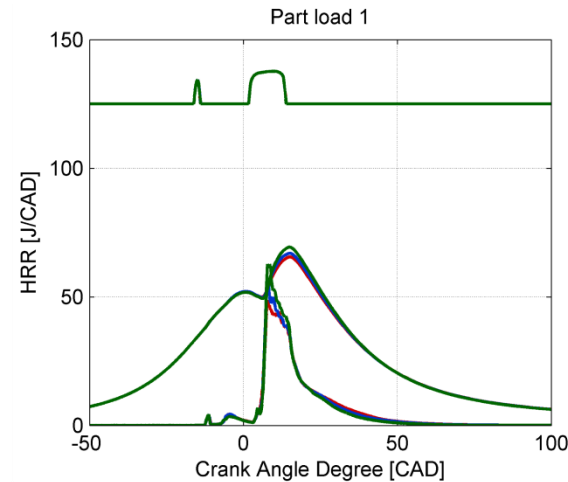
■ Part-load

➤ Enhance the mixing process

- Positive impact on combustion duration (ISFC) and soot emission
- Negative impact on NOx

➤ Promote the premixed combustion stage

- Negative impact on combustion noise particularly at low loads & low speeds

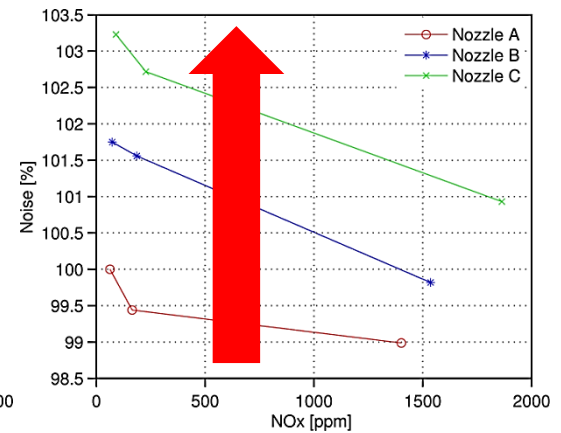
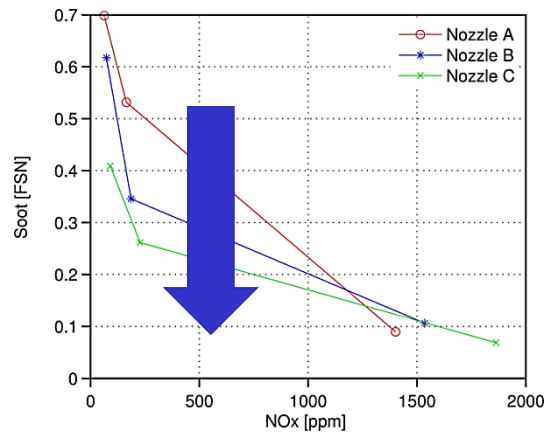
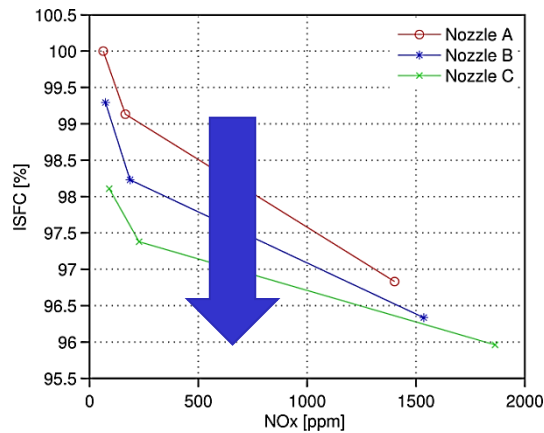


Model application

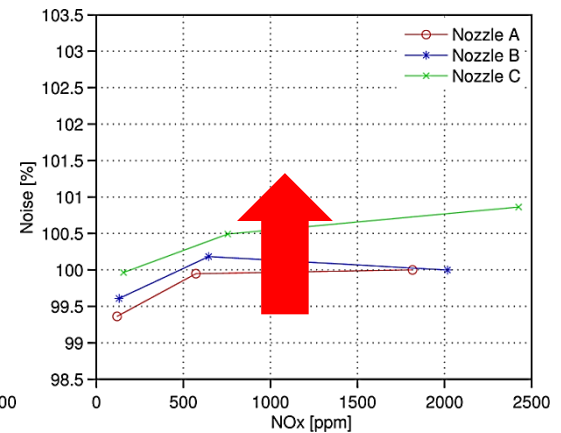
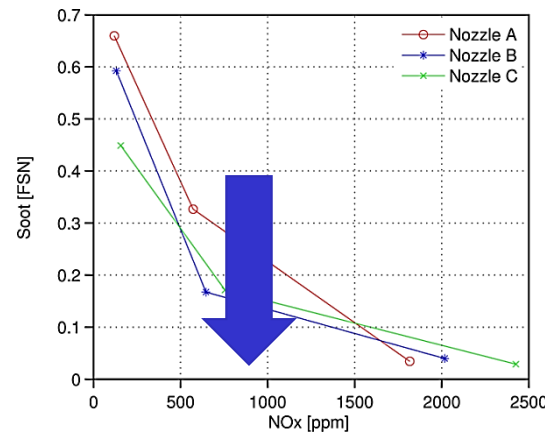
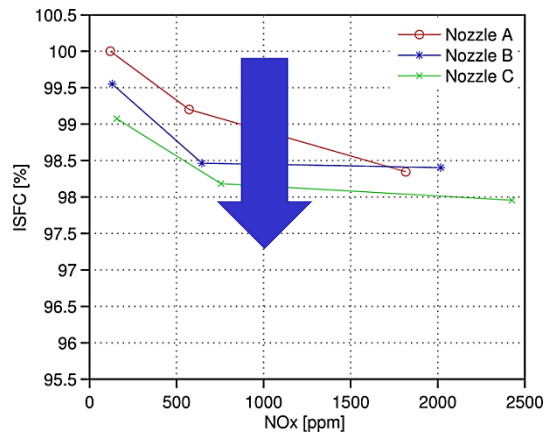
■ Part-load

➤ Better NO_x-soot & NO_x- ISFC trade-offs

Part load 1



Part load 2



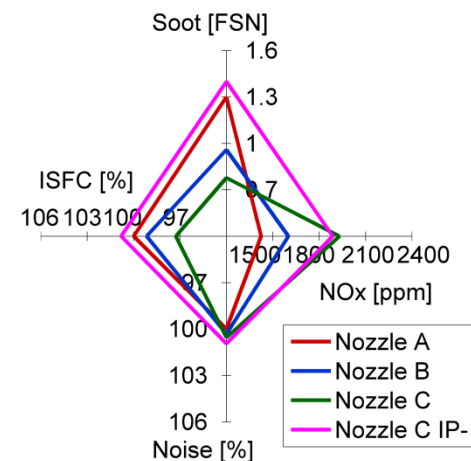
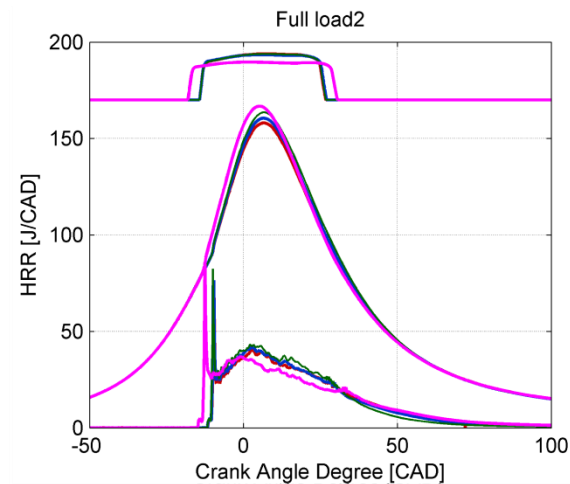
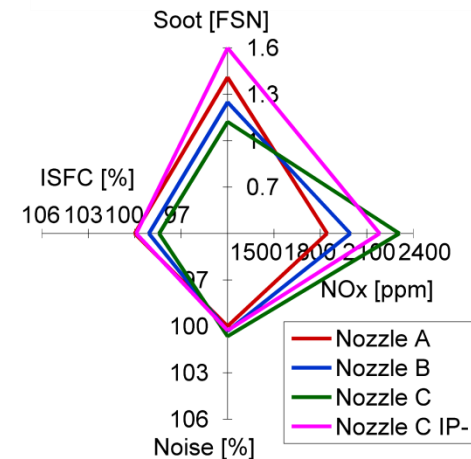
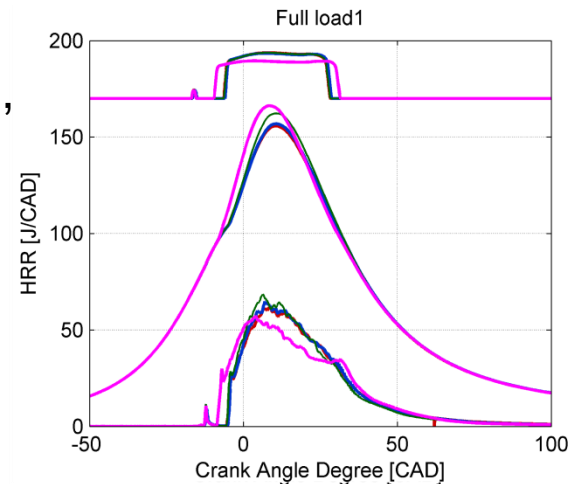
Model application

■ Full-load

➤ Enhance the mixing process, but the impact is slightly noticeable in HRR

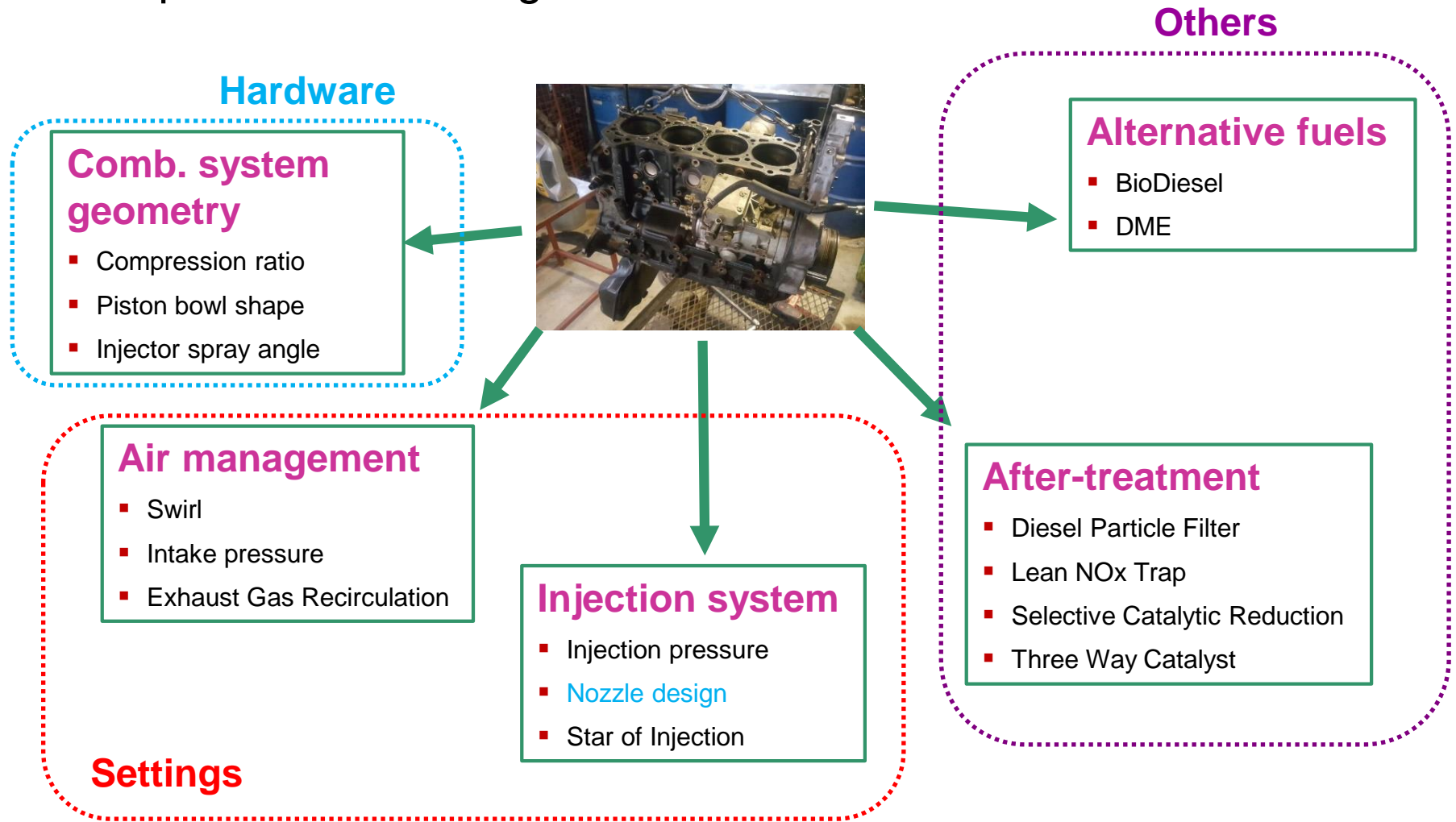
- Positive impact on combustion duration (ISFC) and soot emission
- Negative impact on NOx
- Noise not critical

➤ If Nozzle C is evaluated limiting the injection pressure all benefits are LOST and this configuration is clearly the worst



Framework

■ Optimization strategies for CDC

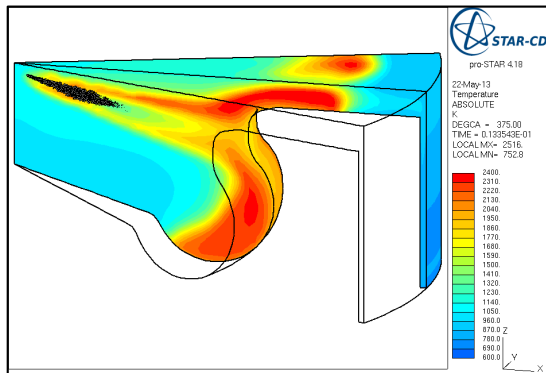


CDC system optimization

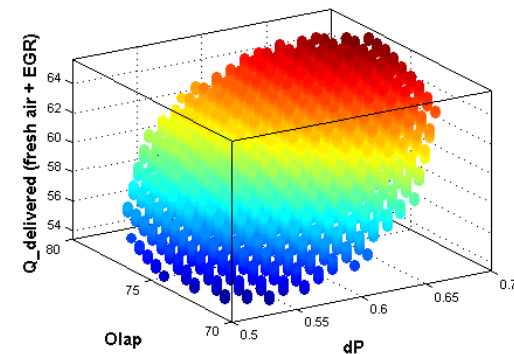
■ Objective:

- Defining the combustion chamber geometry & key engine settings focusing on engine efficiency while keeping emission levels for a medium-duty diesel engine

■ Tools



**Response
Surface
Methods**

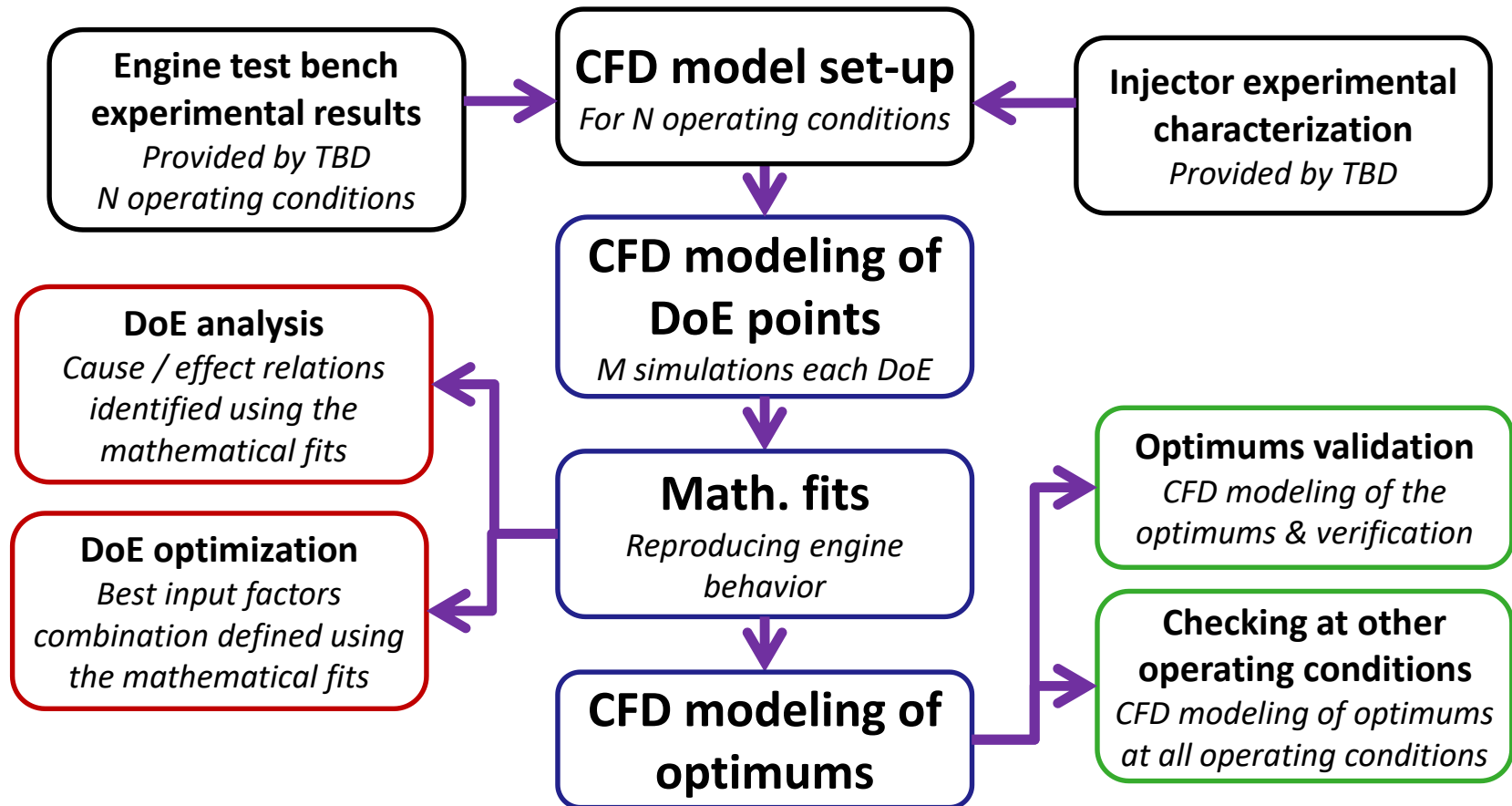


STARCD CFD code

- ✓ Combustion model → ECFM-3z
- ✓ Spray atomization and breakup → Huh-Gosman and Reitz-Diwakar
- ✓ Turbulence model → RNG k- ϵ

Methodology

- Based on Design Of Experiments:

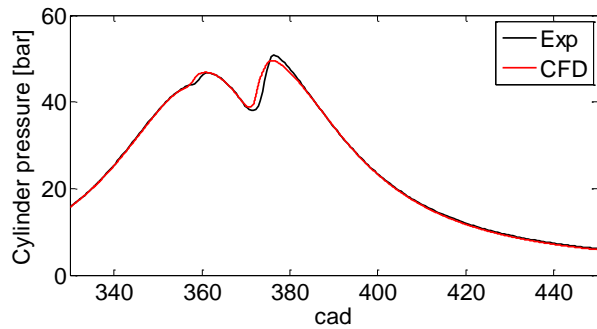


CFD model set-up

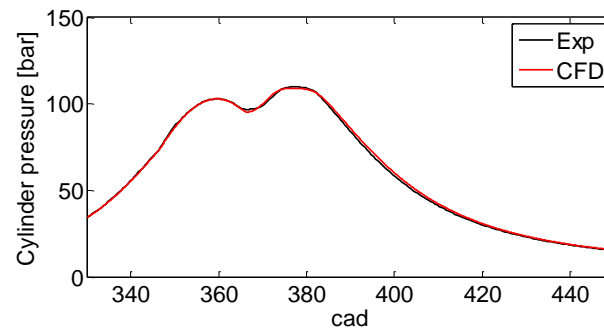
- Overall fair agreement with exp.
 - NOx overprediction at high load/speed, but the quality of CFD was considered suitable

Case		ISFC	IMEP	NOx	Soot
		[g/kWh]	[bar]	[g/h]	[FSN]
1200 rpm	Exp	201.5	6.5	28.6	0.29
	CFD	203.1	6.2	27.6	0.24
1600 rpm	Exp	188.8	17.7	213.3	0.078
	CFD	186.3	18.3	218.6	0.08
1800 rpm	Exp	194.3	24.7	249.16	0.4
	CFD	193.7	24.96	368.4	0.42

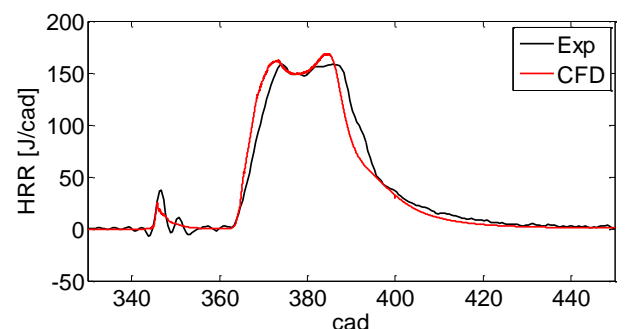
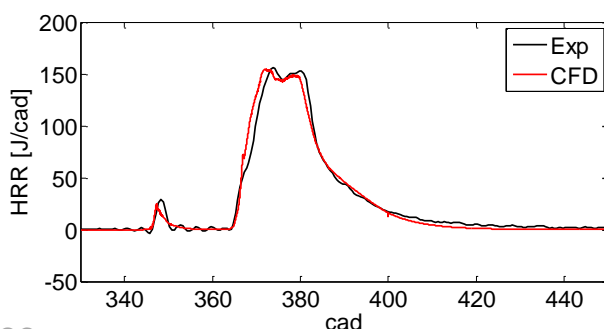
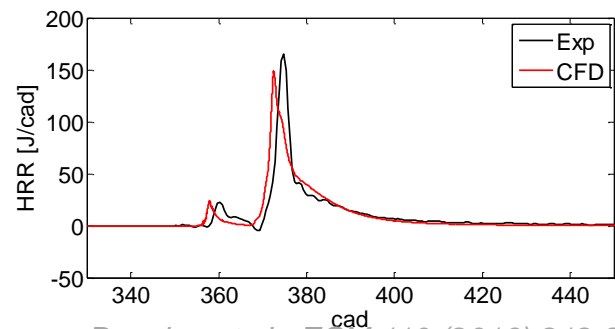
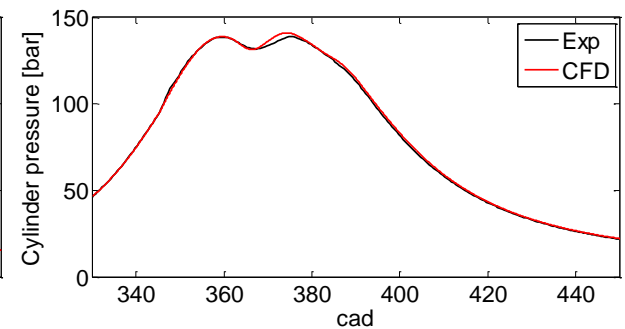
Low load/speed



Medium load/speed



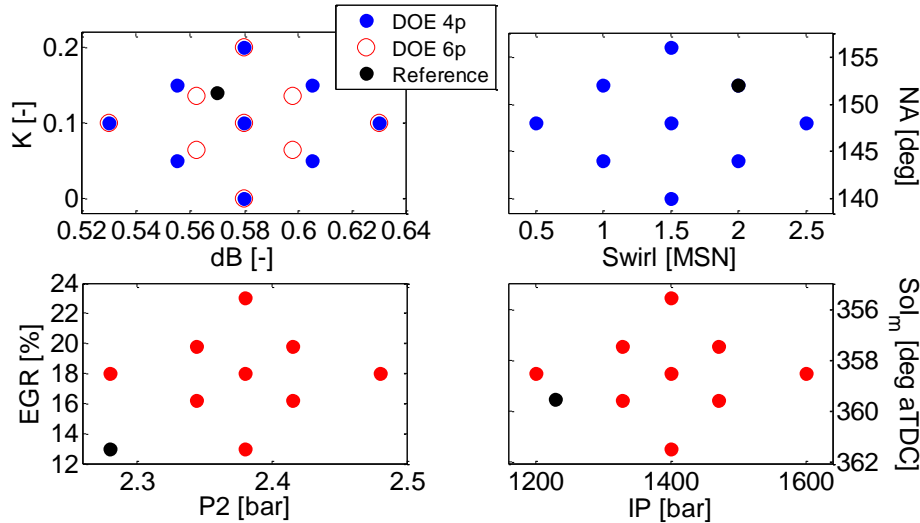
High load/speed



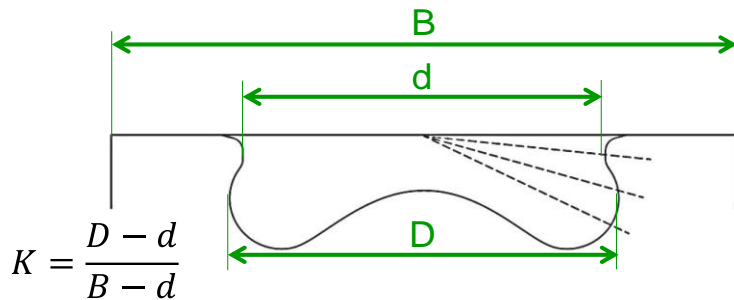
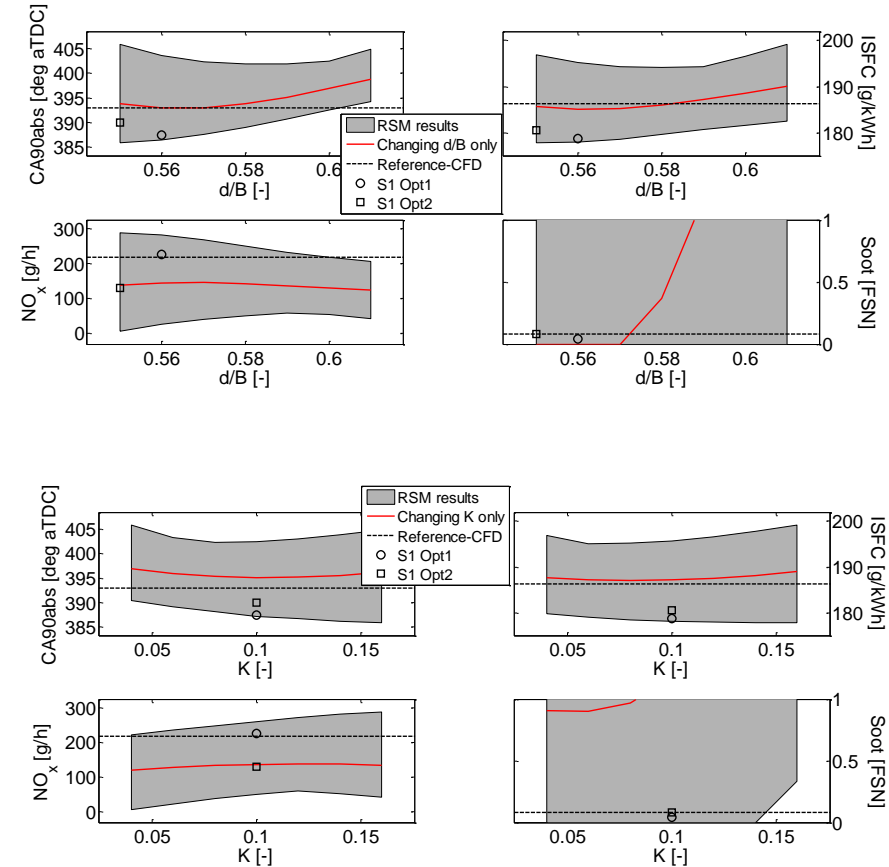
Benajes et al., *ECM 110* (2016) 212-229

DoE - RSM

DoE definition

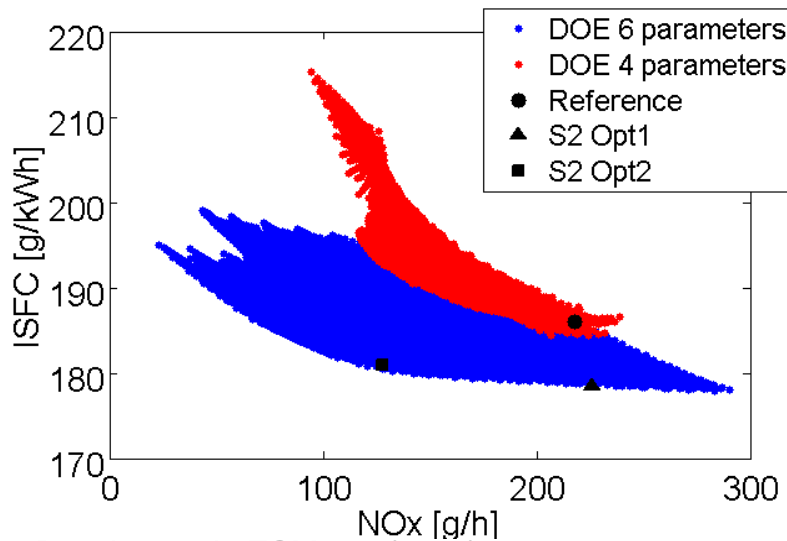


Input factor effect analysis



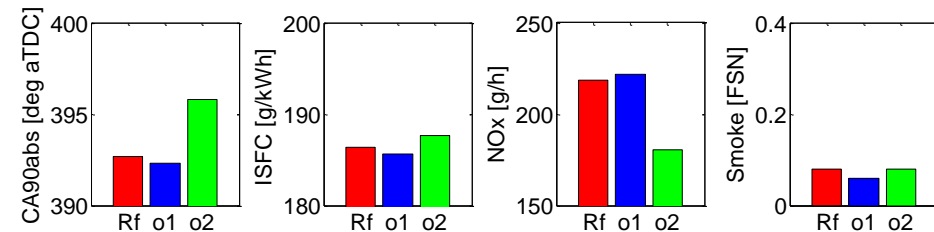
DoE - RSM: Optimum selection and validation

- 2 optimum configuration: min ISFC (o1) and min pollutants (o2)
 - CFD validation of RSM results
- With RSM method it is easy to analyze trade-off between parameters
 - More inputs (settings) → more potential of the combustion system → ISFC-NO_x trade-off still present
 - Geometry, air management and injection settings are not able to break the trade-offs

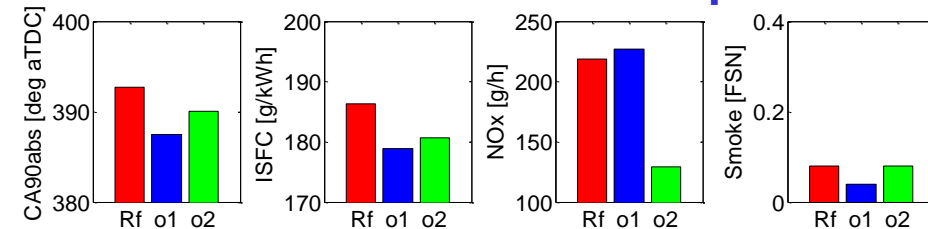


Benajes et al., *ECM 110 (2016) 212-229*

CFD validation DoE 4 p

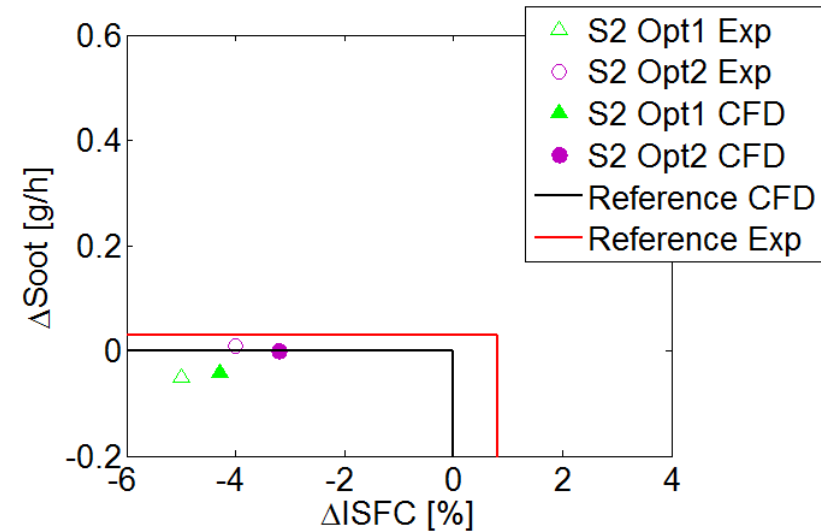
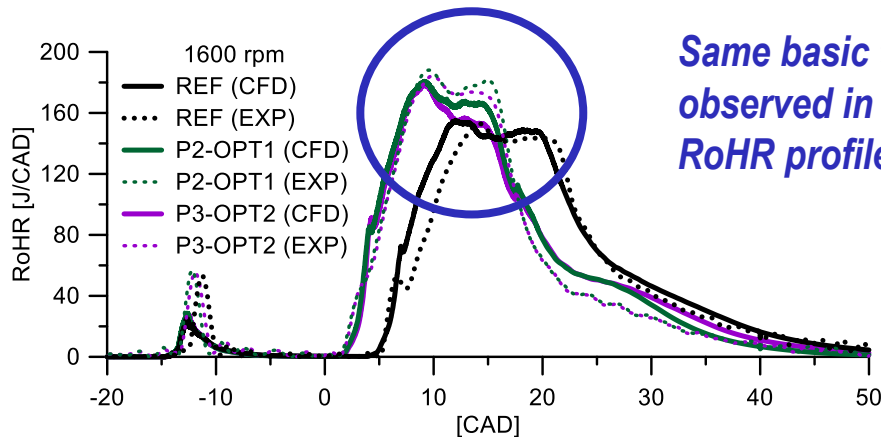
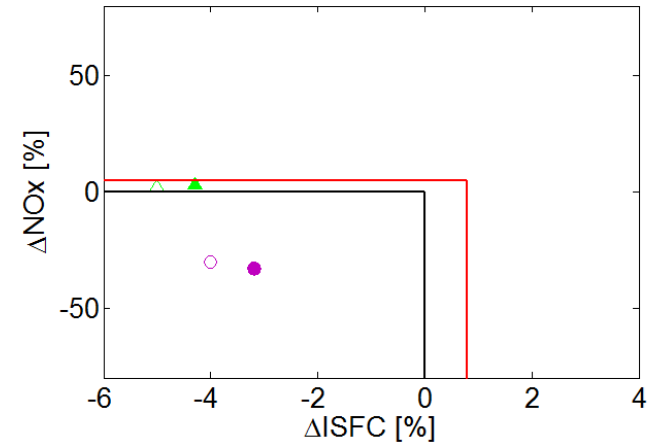
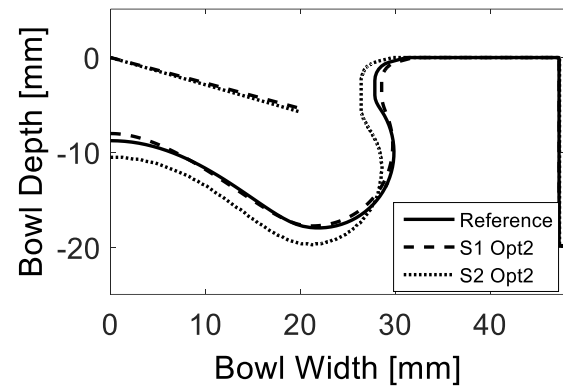


CFD validation DoE 6p



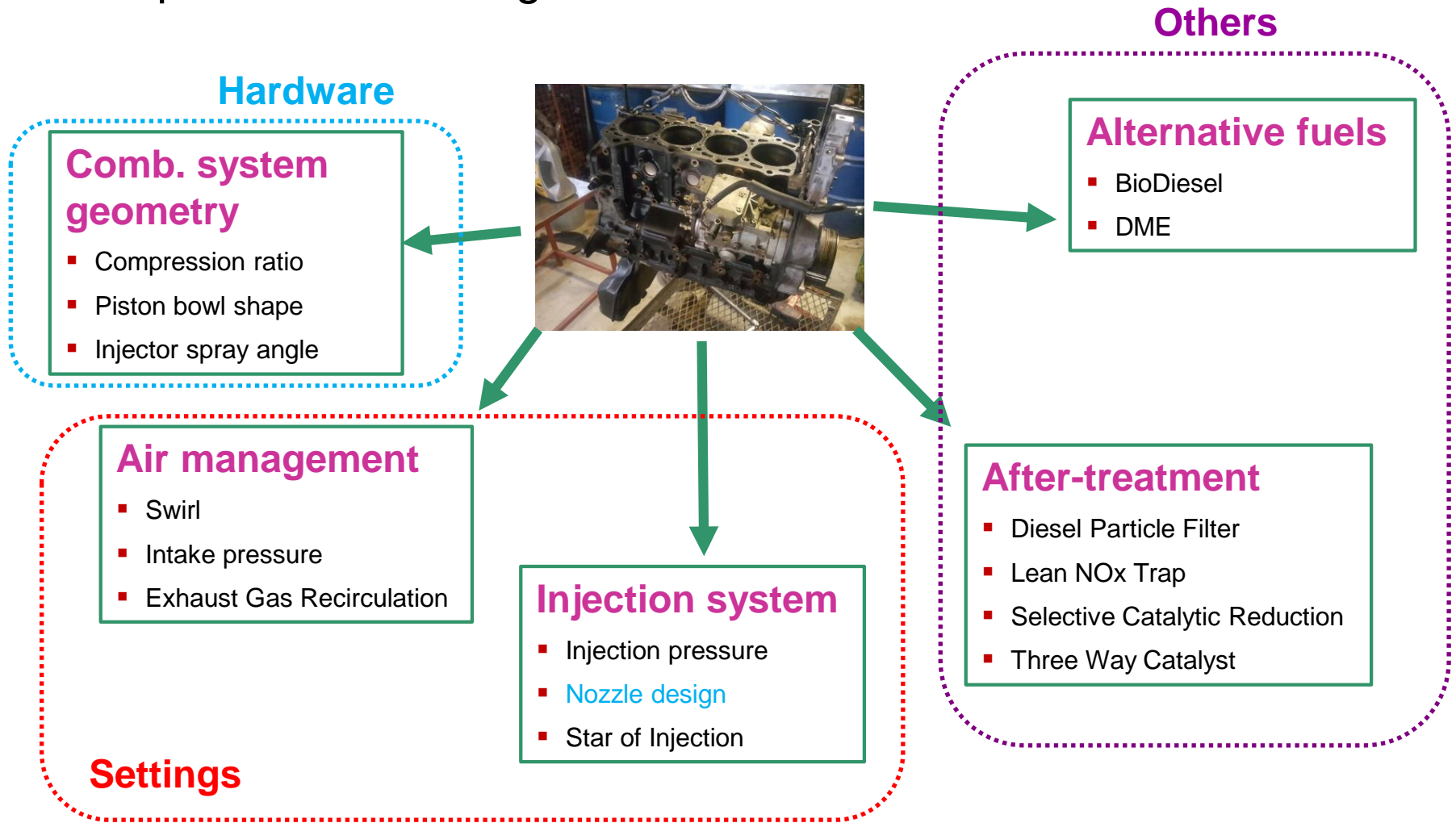
Experimental assessment

- SCE test using machined pistons according CFD results



Framework

- Optimization strategies for CDC



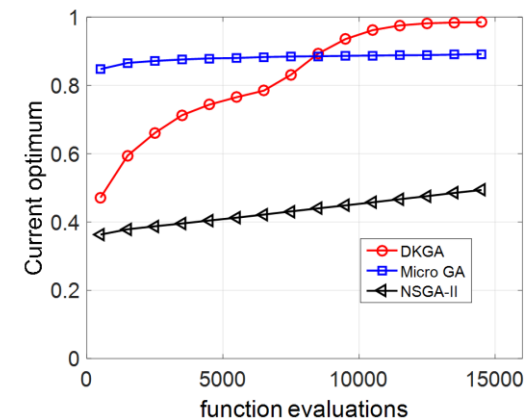
Alternative fuel combustion system

- Background: Main characteristics of the DME fuel
 - Easy to produce from different primary sources
 - Similar combustion properties than diesel fuel
 - Slightly higher cetane number (60), shorter ignition delay
 - Lower heating value (28.8 KJ/kg) but also lower stoichiometric air/fuel ratio (9)
 - Its non-sooting nature opens the possibility of optimization paths
 - It is gaseous in ambient conditions, liquefied by compressing it at 6 bar

- Objective
 - Evaluating in detail the potential of the CDC process using a synthetic fuel with better suited properties than the conventional diesel fuel → Keeping **ALL** the benefits of the CDC improving NOx/soot emissions and efficiency

Methodology & Tools

- Unexplored behavior requires complete combustion redefinition (hardware + settings) → Evolutionary methods better suited for large number of parameter optimization
- Genetic Algorithm
 - Mimics the mechanism of natural selection and evolution: Selection, Crossover and Mutation
 - Very effective with large number of inputs and also when the problem includes non-linear trends
 - Difficult to avoid local optimums
- GA selection → DK-GA (developed at the UWM)
 - Outperformed the other evaluated well-known GA
 - It finds the global optimum
 - It finds it after reasonable number of evaluations



Methodology & Tools

Multicylinder engine

- ✓ 6-cyl TC HDDI engine – 15 liters (2.5 l/cyl)
- ✓ SOI sweep for validation at the target OC

Key characteristics

Operating condition

Bore [mm]	137	Speed [rpm]	1800
Stroke [mm]	171	Fuel mass [Kg/s]	2.2e-2
Comp. Ratio [-]	17:1	IMEP [bar]	18
Injection system	CR	EGR [%]	25
Nozzle holes [-]	6	Intake temp. [K]	333
Hole diam. [mm]	0.214	Boost press. [bar]	3.1
Spray angle [deg]	130	MSN [-]	0.7

CFD platform → KIVA 3v

- ✓ Turbulence model → RNG k-ε
- ✓ Spray model → DDM approach
 - Improved grid dependency: Gas-Jet model
 - Atomization & break-up: KH-RT
 - Improved O'Rourke collision model
- ✓ Combustion model → DIC (SpeedCHEM)
- ✓ DME + NOx chem. model → 29 spec. + 66 reac.
- ✓ Soot model → *Not required*
- ✓ Cores per simulation → 1 core
- ✓ Number of cells → ~35000

} ~20 h/sim

REMARK: Around 25K sim/optimization

Results and discussion

■ Optimization parameters and setup

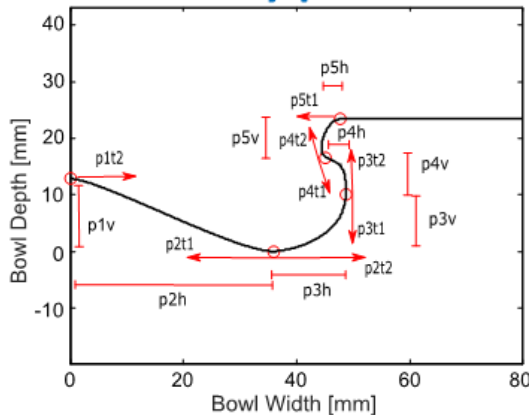
Input parameters

	G1-G4	G5	G6-G15	Dnoz	NA	SOI	IP	EGR	PIVC	swirl
	[-]	[-]	[-]	[μm]	[deg]	[cad]	[bar]	[%]	[bar]	[-]
Min.	0.01	-0.99	0.01	200	45	-35	500	2	2.5	0.1
Max.	0.99	0.99	0.99	350	90	5	2600	62	4	3
	Geometry			Injection			Air management			

Restrictions

NOx	PP	maxPRR
[g/kWh]	[bar]	[bar/deg]
0.268	200	15

Geometry parameters

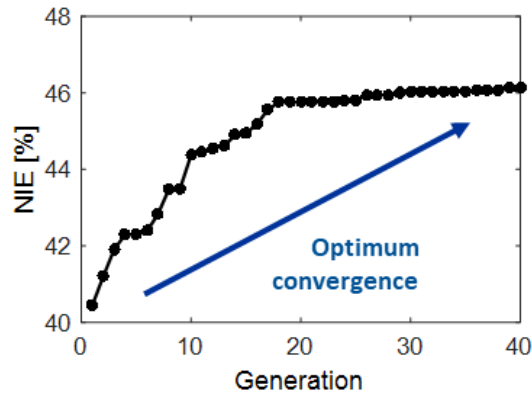


KEY ASPECTS

- ✓ Extended number of input parameters → All key inputs are included → 15 geometry parameters
- ✓ Wide ranges for the selected input parameters
- ✓ Objective function is optimized → high PP, NOx or maxPRR penalizes the objective function output

Results and discussion

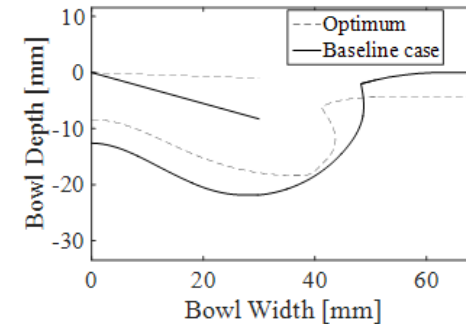
■ Optimum performance description



KEY ASPECTS

- ✓ Geometry changed significantly (keeping CR) → more reentrant, narrower and less depth piston
- ✓ Process converged to an optimum with a 3.3% NIE improvement reducing drastically NO_x
- ✓ All restrictions are satisfied by the optimum

Optimum vs baseline geometry



Optimum settings

	Dnoz [μm]	NA [deg]	SOI [cad]	IP [bar]	EGR [%]	PIVC [bar]	swirl [-]
Baseline DME	300	65	-13	1800	25	3.1	0.7
Opt. Case	300	86.7	-8.19	2500	40	3.25	2.82

Optimum vs baseline outputs

	NIE [%]	maxPRR [bar/deg]	NO _x [g/kWh]	PP [bar]
Baseline DME	42.8	6.1	2.81	193.9
Opt. Case	46.1	6.6	0.26	199.4

Results and discussion

■ Optimum performance description

Energy balance

	G. Ind. Work [J]	Heat Trans. [J]	Exh. Losses [J]	Unburnt Fuel [J]	Pump. Work [J]
Baseline	4854	1926	4215	268	31
Optimum	5207	1779	4183	94	13

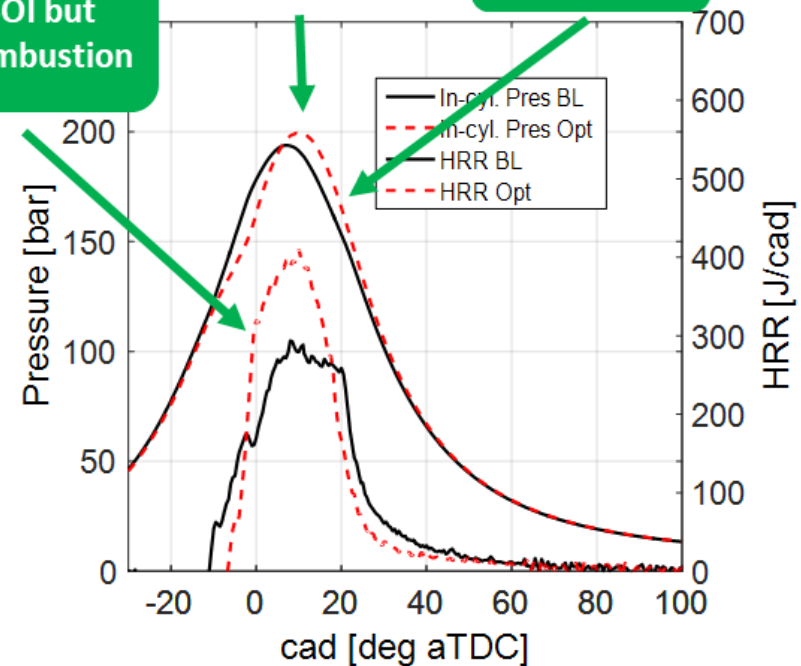
Main differences

KEY ASPECTS

- ✓ Reduced HT → Optimum bowl geometry decreases piston surface area by 20%
- ✓ Better mixing → Faster combustion & higher combustion efficiency (less unburnt HC emissions)

Later SOI but faster combustion

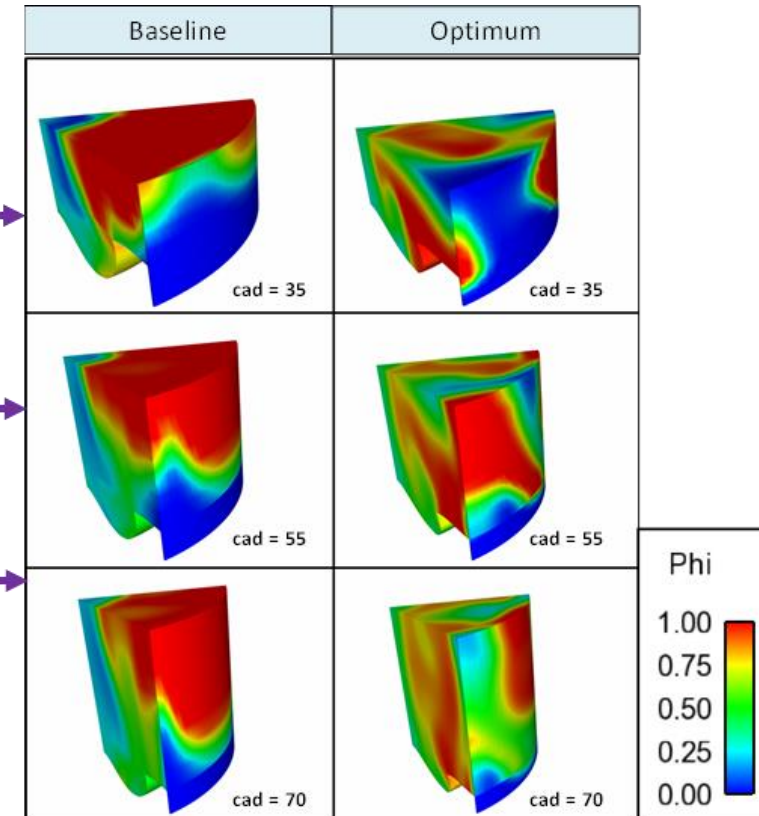
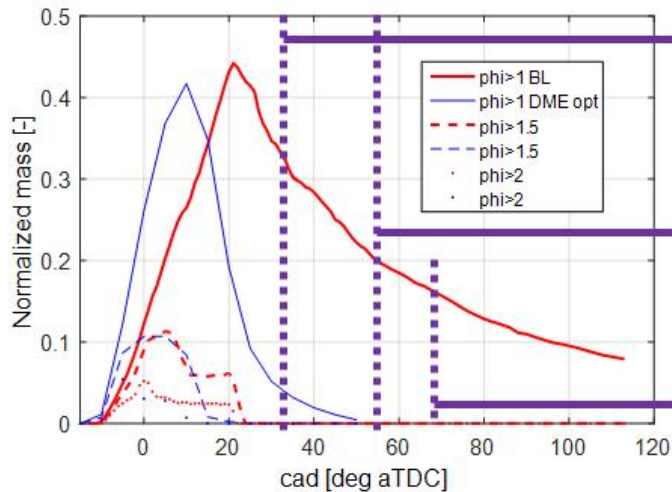
Higher NIE



Results and discussion

■ Optimum performance description

Local equivalence ratio evolution



KEY ASPECTS

- ✓ Better mixing mainly promoted by the higher injection pressure & better suited internal aerodynamics

Results and discussion

■ Optimization path analysis

Reduces HT increasing GIE

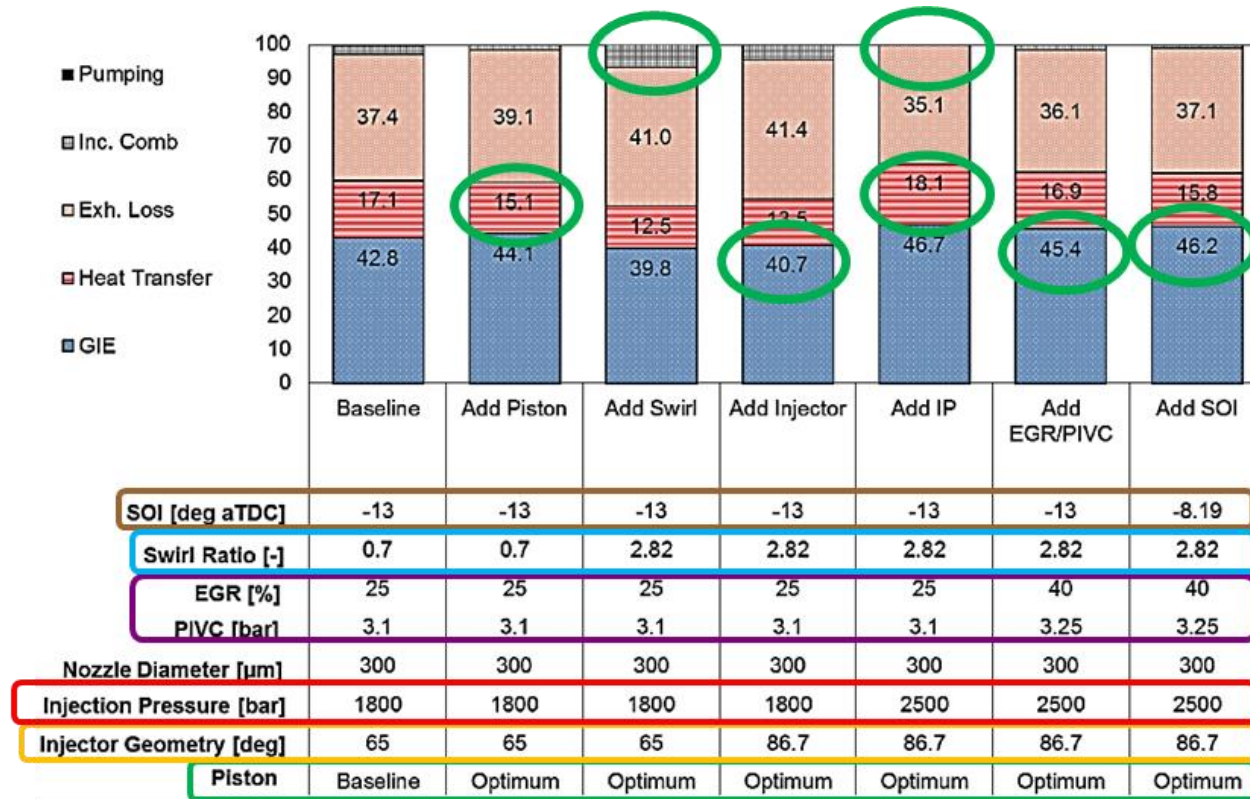
Worsens spray-to-spray interaction decreasing GIE

Improves mixing and then increases GIE (low effect)

Improves mixing and then increases GIE (high effect)

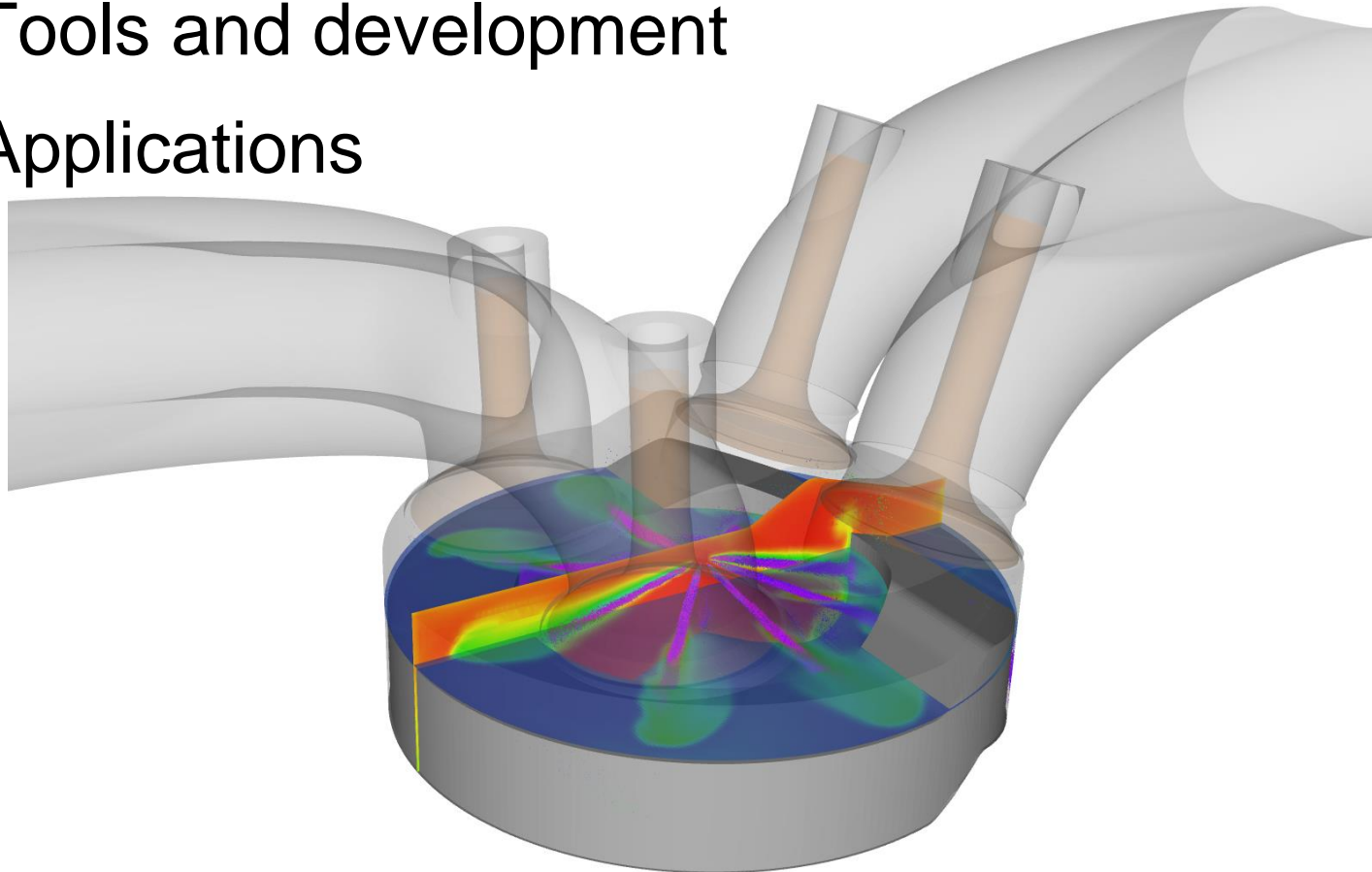
NOx control but PIVC limited by pumping losses, GIE decreases

Further improves GIE until reaching the PP limit



CONTENTS

- Background and approach
- Tools and development
- Applications



ACKNOWLEDGEMENTS

- CFD combustion group members and collaborations
 - Prof. JM García-Oliver and Prof. R. Novella
 - J. Gomez-Soriano, E.J. Perez, A. Hernández-Lopez, L. Pachano, ...
 - Dr. A. Pandal & Dr. J.F. Winklinger (former CMT PhD Students)
- CMT combustion research manager Prof. J. Benajes

Gracias por su atención !