Technische Universiteit **Eindhoven** University of Technology

Multiphase and Reactive Flows Group

3rd Two-day Meeting on IC Engine Simulations Using OpenFOAM® Technology

22-23 Feb 2018 - Milano

Incorporation of Flamelet Generated Manifold Combustion Closure to OpenFOAM and Lib-ICE

Amin Maghbouli

Bart Somers

Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions

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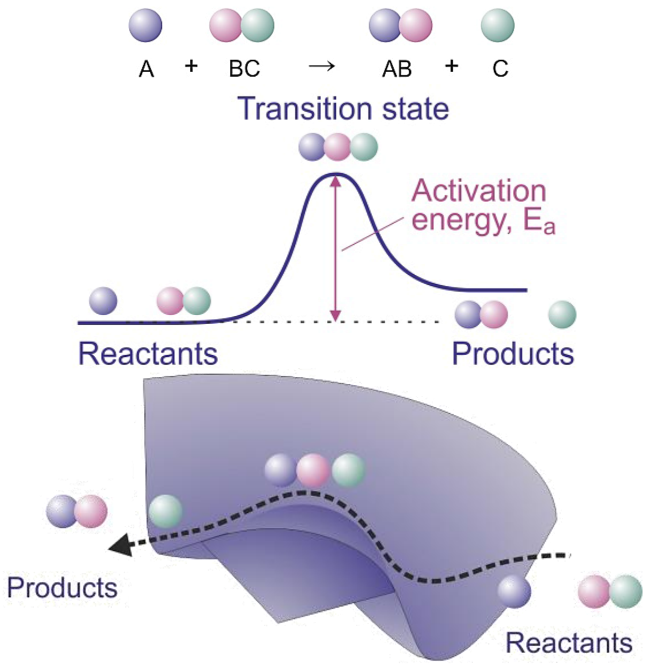
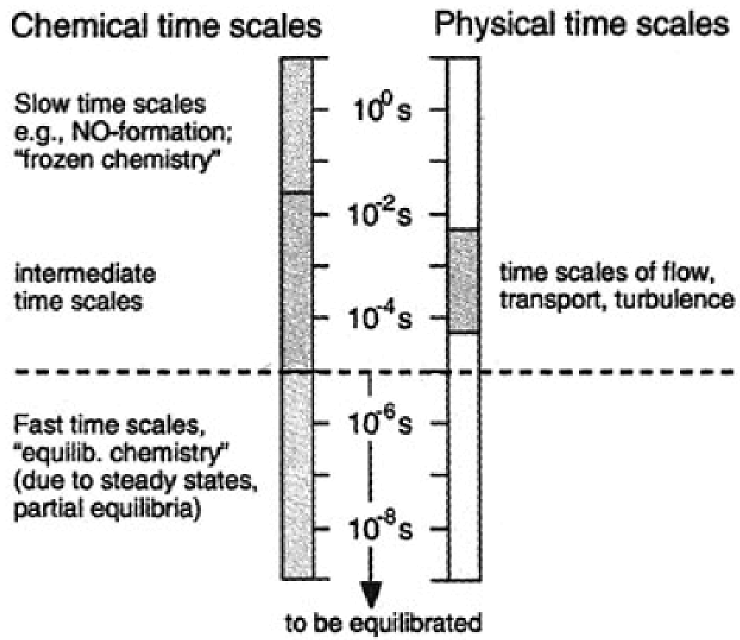
Introduction to Chemistry Reduction Methods

Chemical Kinetics of Reactive Flows





- Result in system of stiff ODE and solution for reaction rates requires specific mathematical algorithms.
- Hinders prospective CFD simulations of reactive flows.

Introduction to Chemistry Reduction Methods

Chemistry Tabulation vs on-the-fly Chemistry

Chemistry Tabulation

- No integration for Chemistry
- Look up routines for updating sources

on-the-fly Chemistry

- Direct integration for chemistry
- Sources update after chemistry integration

Progress Variable approach

Flame Types:

- *Perfectly Stirred Reactor*
- *Approximated Diffusion Flemelet*
- *Flamelet Generated Manifolds*

Developed at TU/e

Contents:

FGM Implementation to OpenFOAM and Lib-ICE

Flamelet Generated Manifolds

www.fgm-combustion.org

CHEM1D: 1D flamelet solver code:

- Adaptive gridding
- Implicit solver
- Timestepper (real /false)
- Flexible inlet composition
- CHEMKIN III compatible
- Thermal diffusion
- Transport modelling
- Unity Lewis numbers
- Constant Lewis numbers
- Different Flame Types
- Mixture average

The Simulation of Flat Flames with Detailed and Reduced Chemical Models, Bart Somers

FGM Implementation to OpenFOAM and Lib-ICE

Tabulation of counter flow flamelets for Reacting Sprays

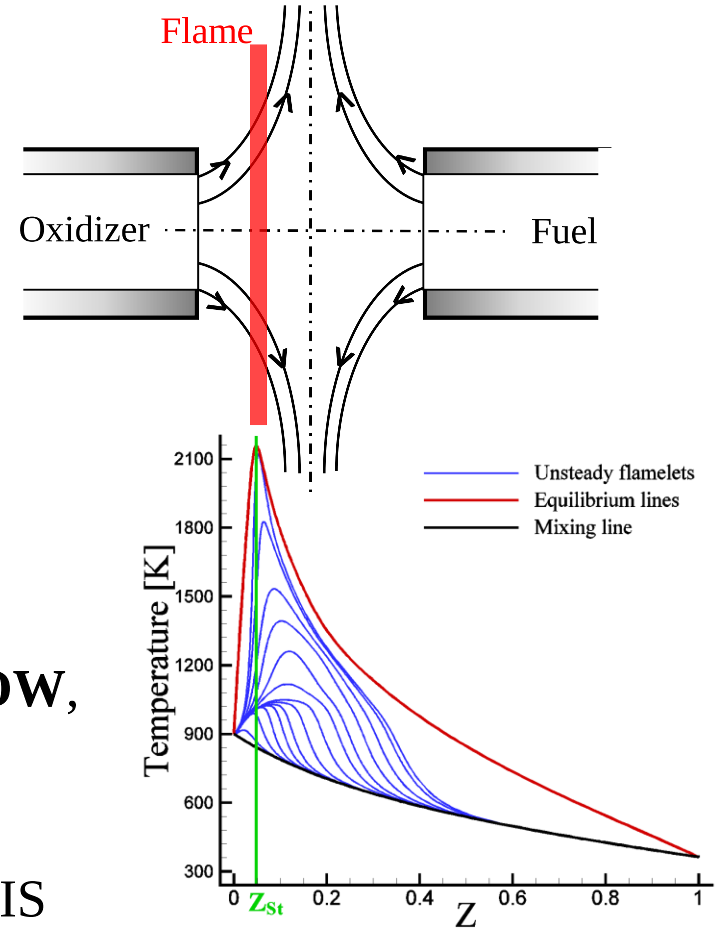
Reaction Space – flamelet solver

- CHEM1D solver code was used for flamelet generation.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\rho x} = -\rho K$$

$$\frac{\partial \rho Y_n}{\partial t} + \frac{\partial \rho u Y_n}{\rho x} = \frac{\partial}{\partial x}\left(\rho D \frac{\partial Y_n}{\partial x}\right) + \dot{\omega}_n - \rho K Y_n$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u h}{\rho x} = \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial x}\right) - \rho K h$$



- CHEM1D:

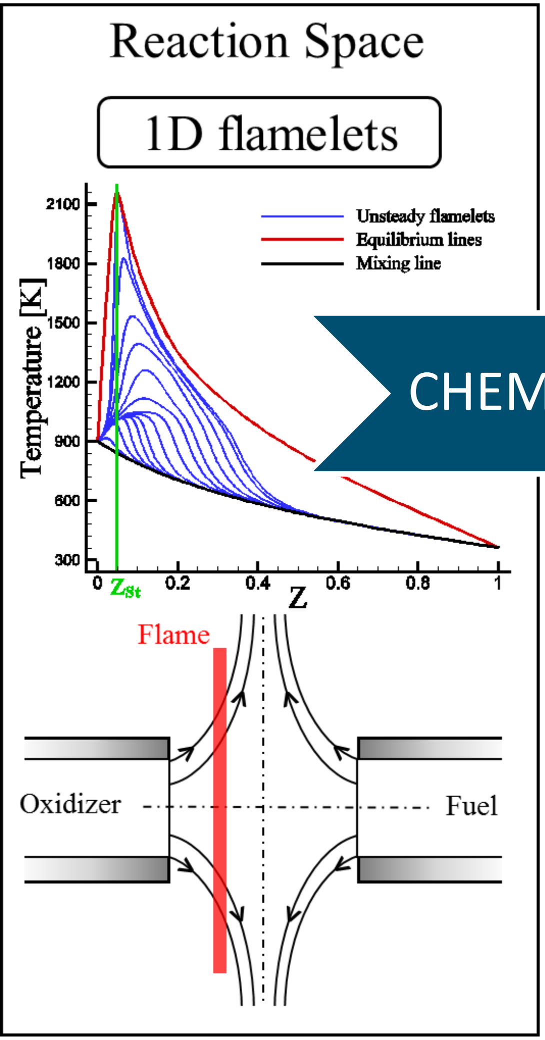
Includes different **Flame Types**:

FREE, BURNERSTABILIZED, **COUNTERFLOW**, BIO, and …

Transport:

UNITY LEWIS, CONSTANT/VARIABLE LEWIS

FGM Implementation to OpenFOAM and Lib-ICE



bash script for parallel flamelet generation

Frozen Flamelet Method, FFM for IC Engine applications

CHEM1D → MATLAB scripts → FGM table

Needed format for table data

CFD

Table dimensions parametrization & interpolation

Variable definition & calculation

FGM Implementation to OpenFOAM and Lib-ICE

Lib-ICE:

- Flamelet CFD solver for reacting spray and IC engine
- Source code for table dimensions and data handling

Dimensions for tabulation of chemistry can be:

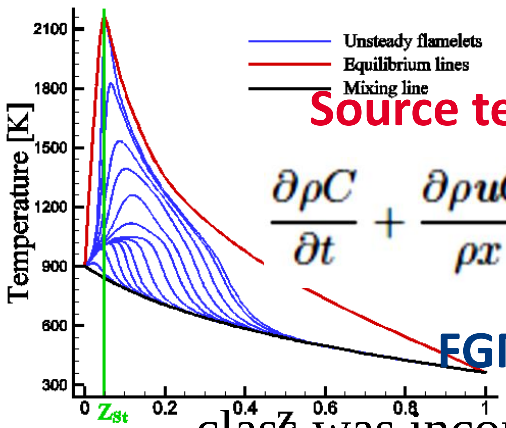
4D Tables for IC Engines

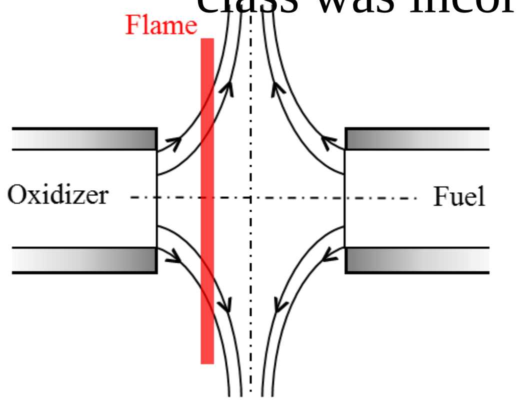
Progress variable	c	1D
Mixture fraction	Z	2D
Unburned Temperature	T_u	3D
Pressure	p	4D
Segregated Mixture Fraction	Z_2	
Segregated Progress variable	c_2	6D
Scalar Dissipation Rate	χ	7D

FGM Implementation to OpenFOAM and Lib-ICE

Reaction Space

1D flamelets





1

Tabulated Chemistry

4D-FGM

Source term from FGM tables

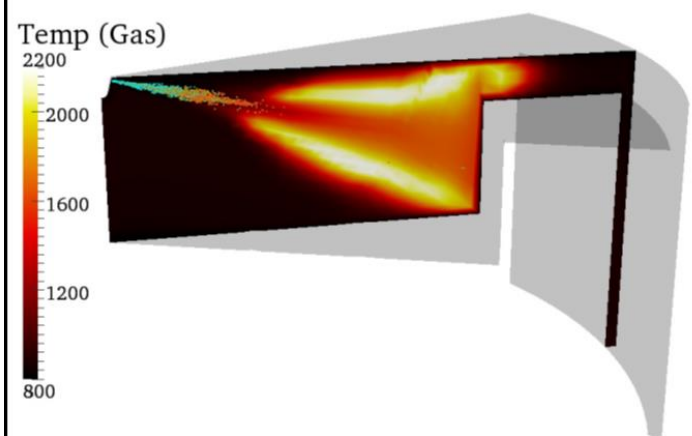
$$\frac{\partial \rho C}{\partial t} + \frac{\partial \rho u C}{\rho x} = \frac{\partial}{\partial x}\left(\frac{\mu_t}{Sc_t}\frac{\partial C}{\partial x}\right) + \boxed{\rho \dot{C}}$$

FGMFlameletLibrary

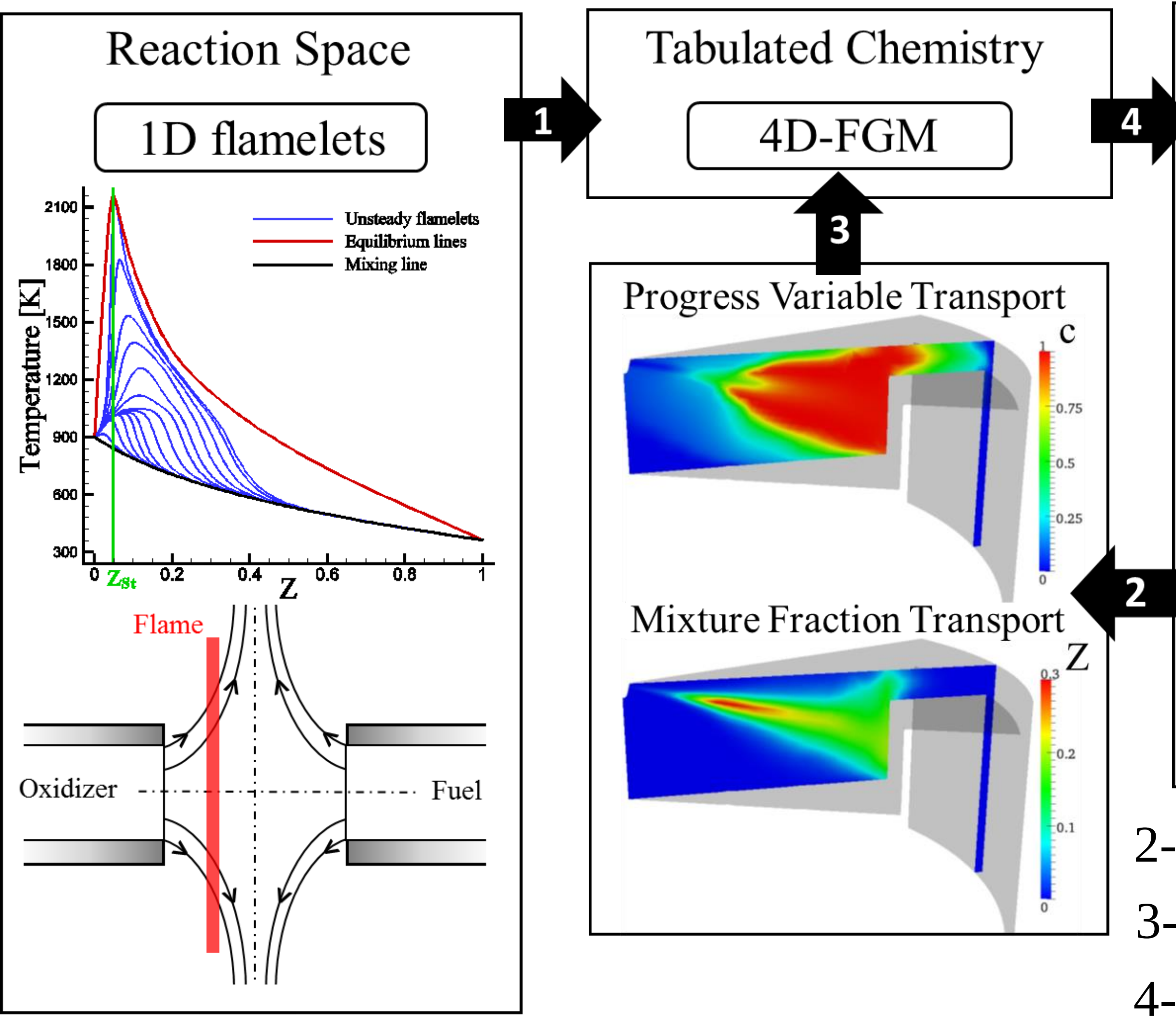
class was incorporated to the Lib-ICE source

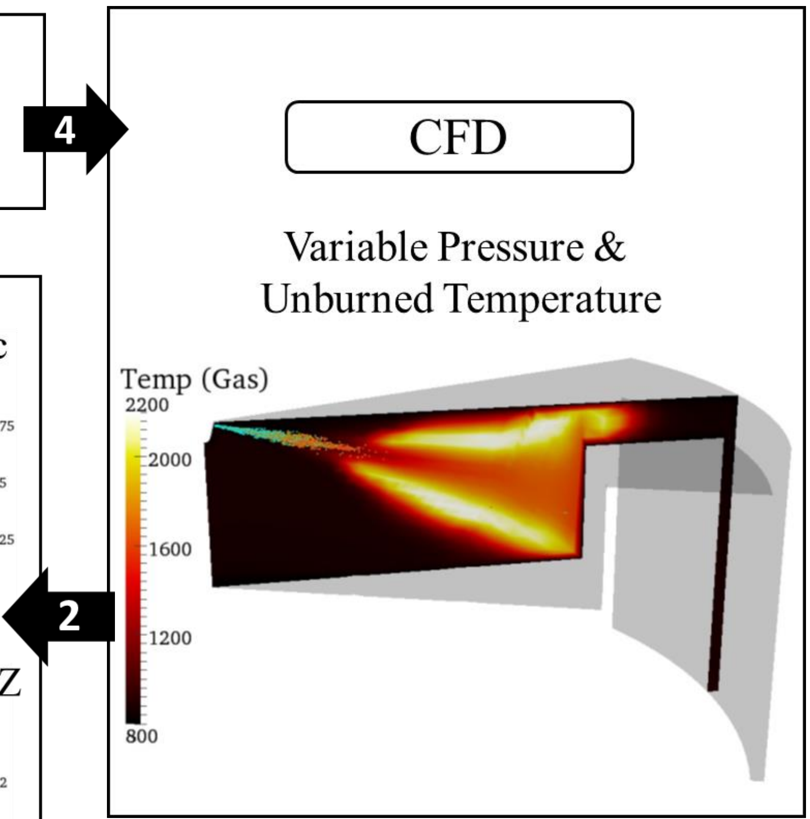
CFD

Variable Pressure & Unburned Temperature



FGM Implementation to OpenFOAM and Lib-ICE





2- Transport of **c** and **Z** Fields

3- **c, Z, P, Tu** from CFD to Table

4- **cdot** from Table to Update CFD

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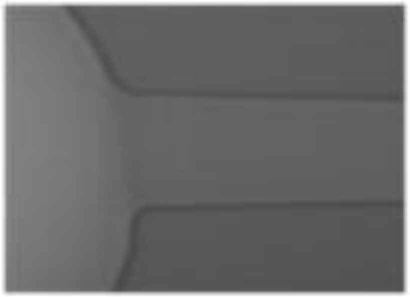
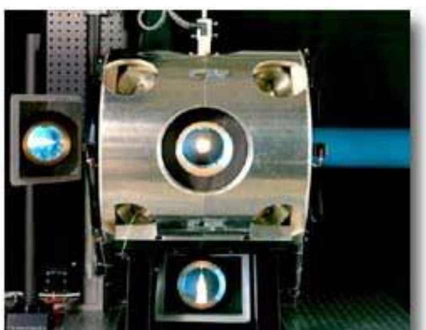
Case Study: Constant Volume Vessel | ECN Spray A

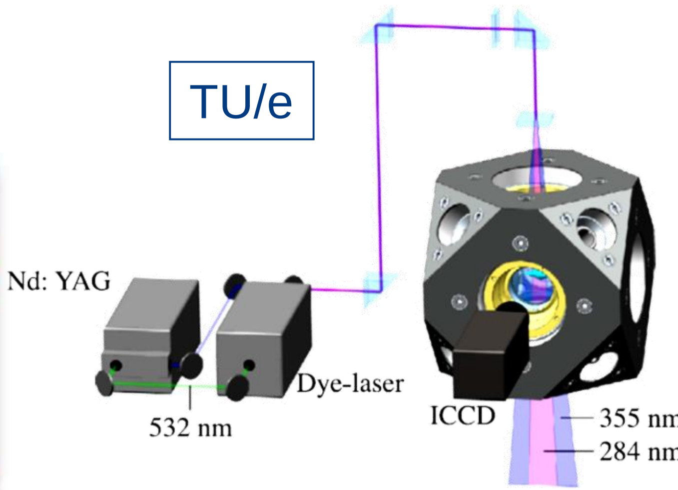
Experimental configuration



Sandia



TU/e



ECN

Specifications for Spray A of the ECN	
Fuel injector	Bosch
Orifice diameter	0.090 mm
Nozzle K factor	K = 1.5
Nozzle shaping	Smoothed
Mini-sac volume	0.2 mm^3
Discharge coefficient	$C_d = 0.86$
Number of holes	single hole
Orifice orientation	Axial

Large set of experimental and numerical data for non-reacting and reacting operating conditions

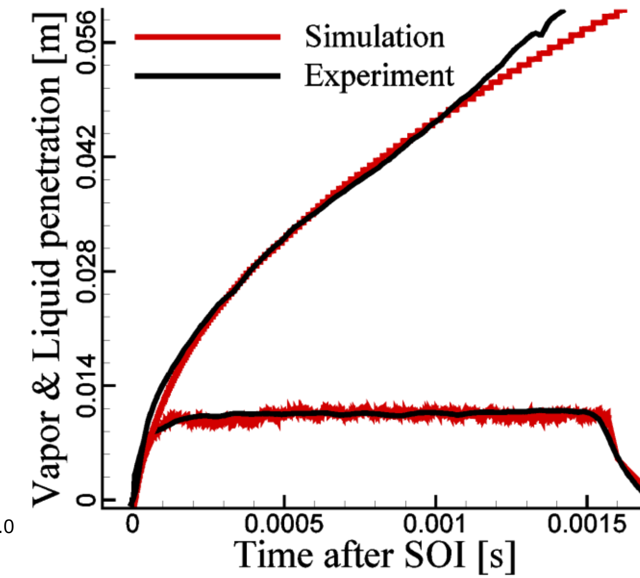
Non-reacting: Liquid/vapor pen. and Mixture Fraction distribution

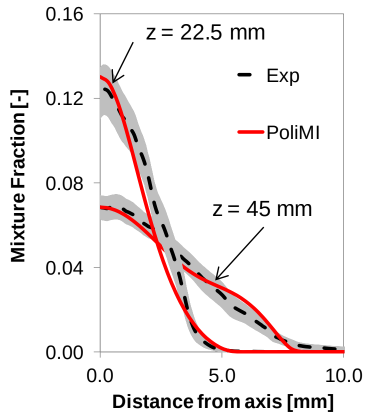
Reacting: Ignition delay and Flame Lift-off

Case Study: Constant Volume Vessel | ECN Spray A

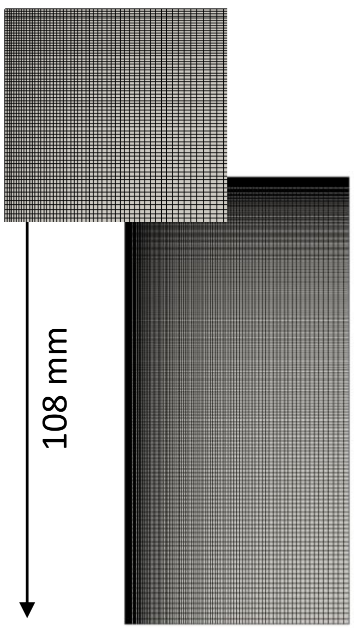
Non-reacting: Liquid/vapor penetration and Mixture Fraction distribution

(RANS)

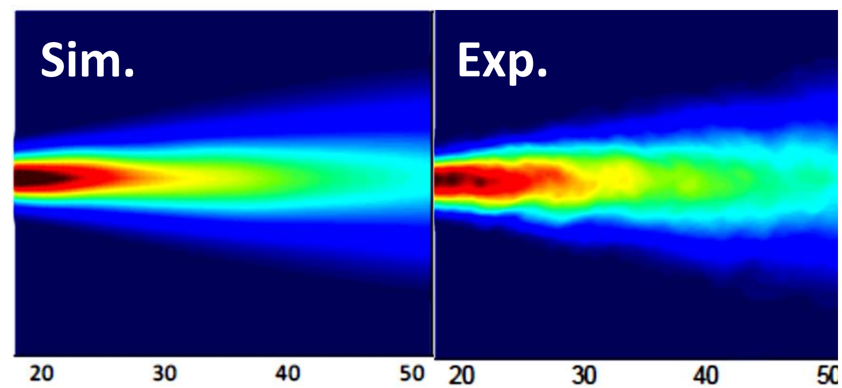




Baseline operating condition

2D computational mesh	
	**CFD setup** • Injection: blob • Breakup: KHRT • Evaporation: Spalding • Turbulence model: standard k-ε with modified C_1 **Test conditions** • Fuel n-dodecane • Nozzle diameter: 90 μm • p_{inj}: 150 MPa • T_{amb}900 K • ρ_{amb} : 22.8 kg/m^3

Mixture Fraction



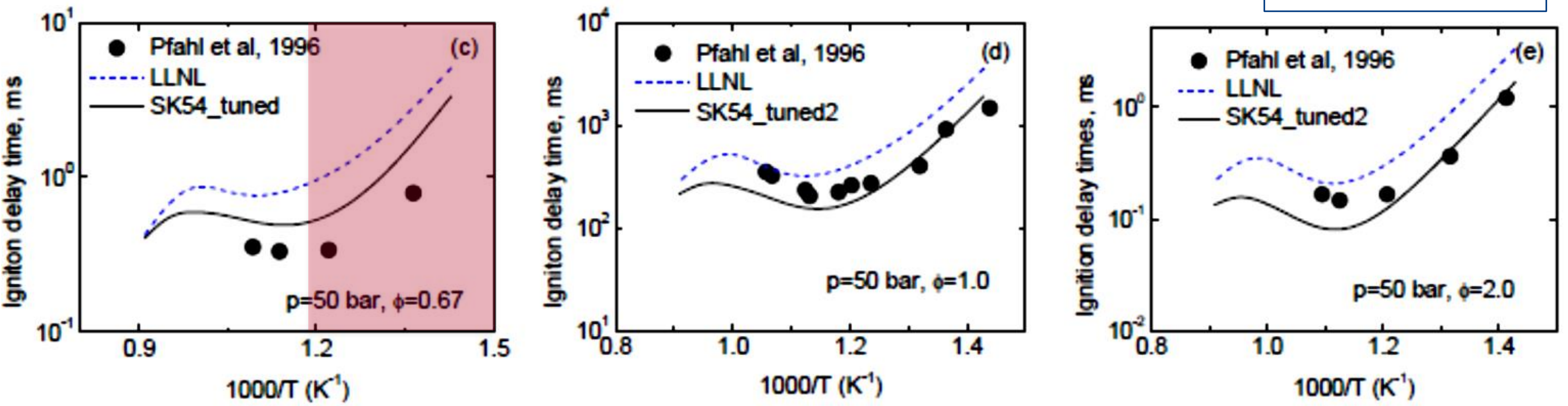
Case Study: Constant Volume Vessel | ECN Spray A

n-dodecane Chemistry:

Mechanism of Yao et al. was used.

54 species and 269 reactions

Yao et al.
9th U. S. National
Combustion
Meeting



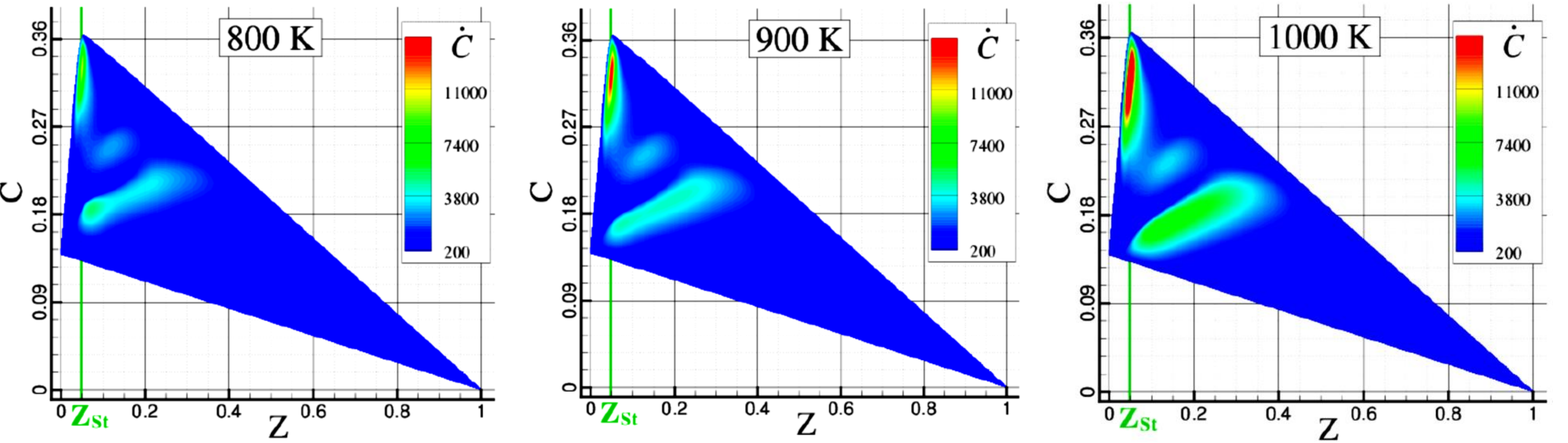
Case Study: Constant Volume Vessel | ECN Spray A

FGM: Table dimensions and progress variable definition

Spray A ambient composition

$$C = Y_{HO_2} + Y_{CH_2O} + Y_{H_2O} + Y_{CO_2} + Y_{CO}$$

Parameter	Range	No. of discretization points
Progress Variable	$0 < c < 1$	500
Mixture Fraction	$0 < Z < 1$	500
Unburned Temperature [K]	$750 < T_u < 1100$	6
Pressure [bar]	$50 < p < 80$	3

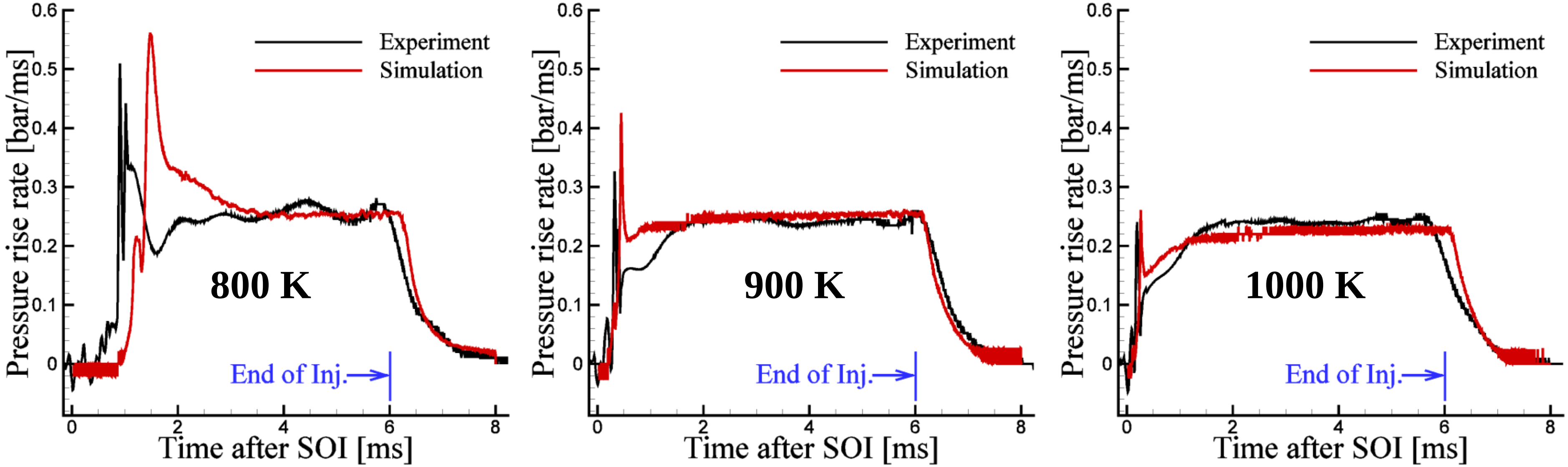


TU/e Technische Universiteit Eindhoven University of Technology

Case Study: Constant Volume Vessel | ECN Spray A

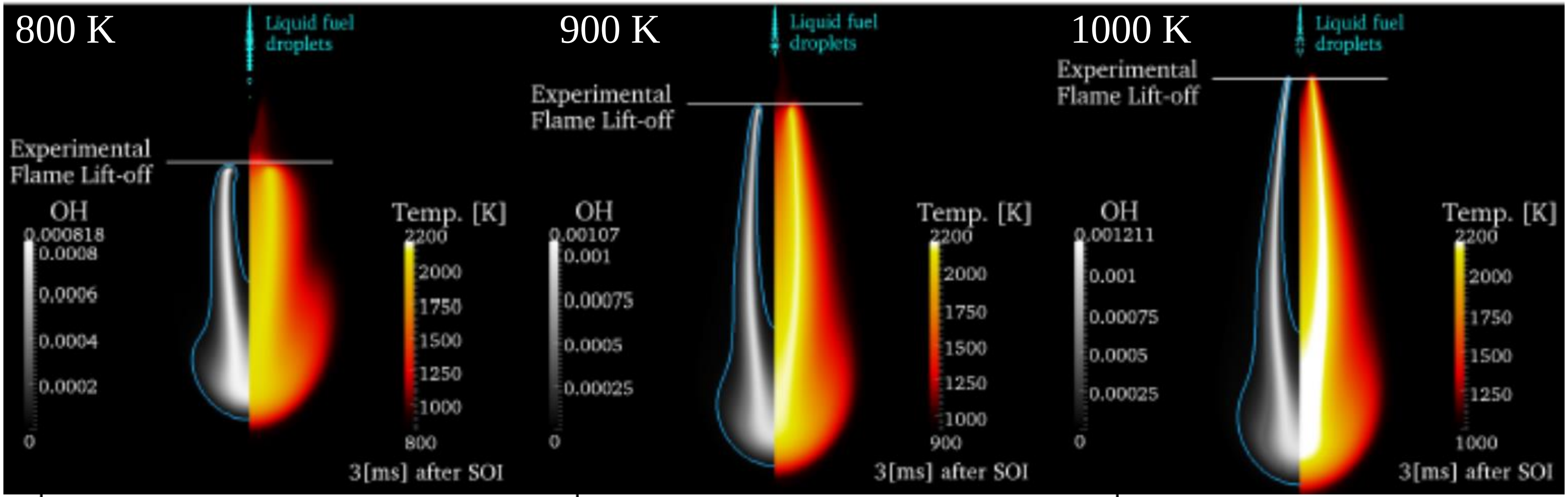
Reacting: Ignition Delay, PRR, Flame Lift-off

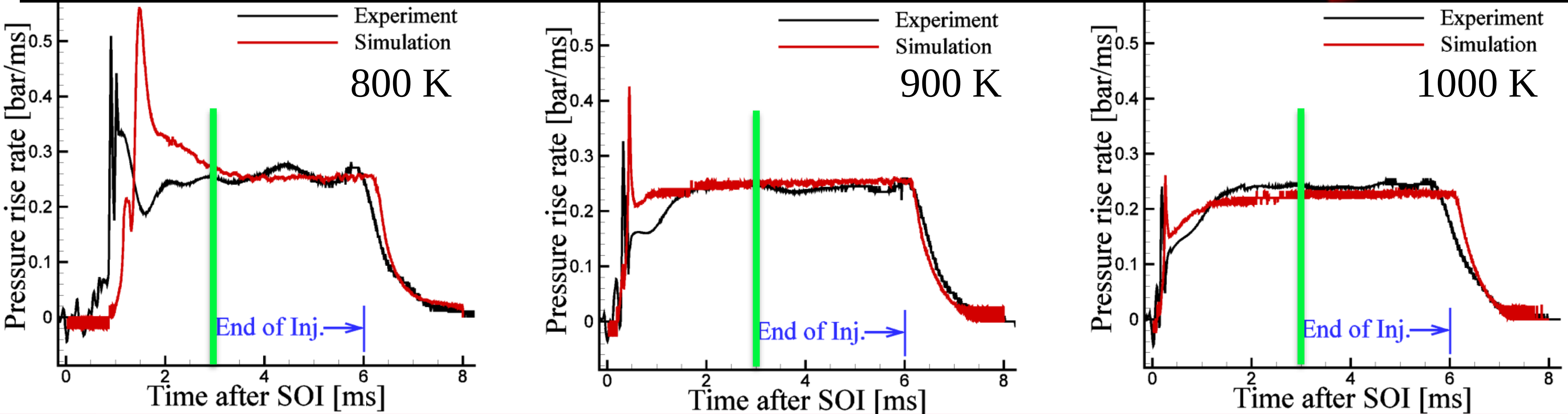
Ambient temperature [K]	800	900	1000
Ignition delay [ms] Simulation	0.91	0.45	0.25
Experiment	**0.85**	**0.41**	**0.24**
Flame lift-off [mm] Simulation	25.1	16.5	11.7
Experiment	**26.2**	**16.7**	**12.2**



Case Study: Constant Volume Vessel | ECN Spray A

Reacting: Ignition Delay, PRR, Flame Lift-off at 3 CAD ATDC





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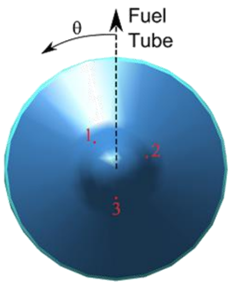
Case Study: Light Duty Diesel Engine | ECN Spray B

Experimental configuration

SAE 2016-01-0743

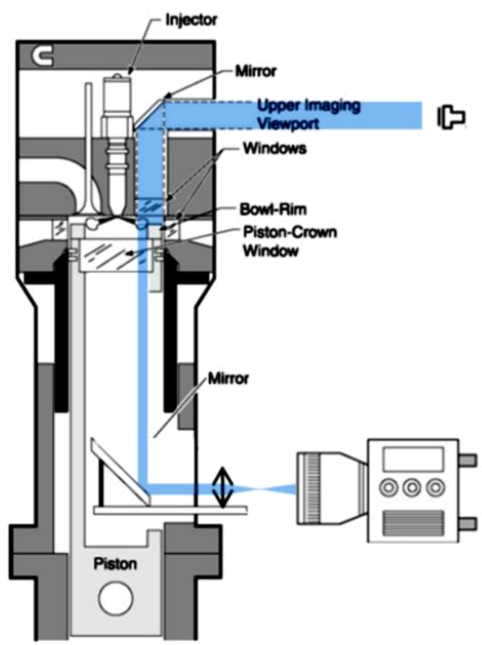
Spray B – Bosch injector

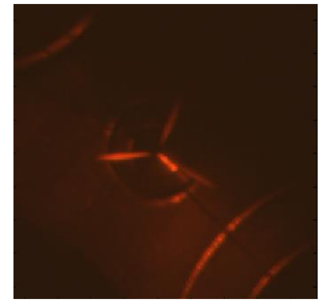


Injector type	#211199 Bosch Spray B
Hole sizes, #1, 2, 3	90.9 μm, 91.7 μm, 90.9 μm
Nominal included angle	145°
Nozzle shaping	Smoothed
Discharge coefficient	C_d = 0.86
Hole angular position	#1 36.4°, #2 -62.3°, #3 180°

Sandia Optical Engine

Intake valves	2
Exhaust valves	1
Swirl ratio	0.5
Bore × Stroke	13.97 × 15.24 cm
Bowl width × depth	9.78 × 1.55 cm
Displacement	2.34 L
Compression ratio	11.22 : 1
Connecting rod length	30.48 cm

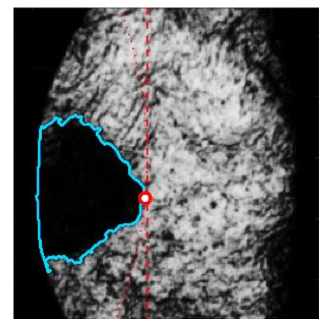




Liquid Penetration Length

Mie scattering

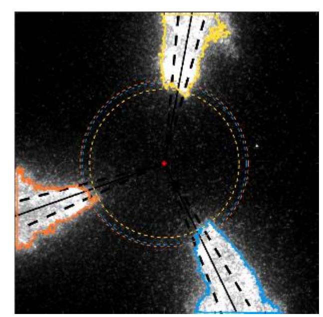
- Color Phantom v611
- Frame rate 67kHz,
- Exposure: 14us
- Lens =85mm f/1.4



Vapor Penetration Length

Schlieren

- Phantom v71
- Frame rate: 25kHz
- Exposure: 19us
- Lens: 105mm f/2.5



Flame Lift-off Length

*Chimiluminescence OH**

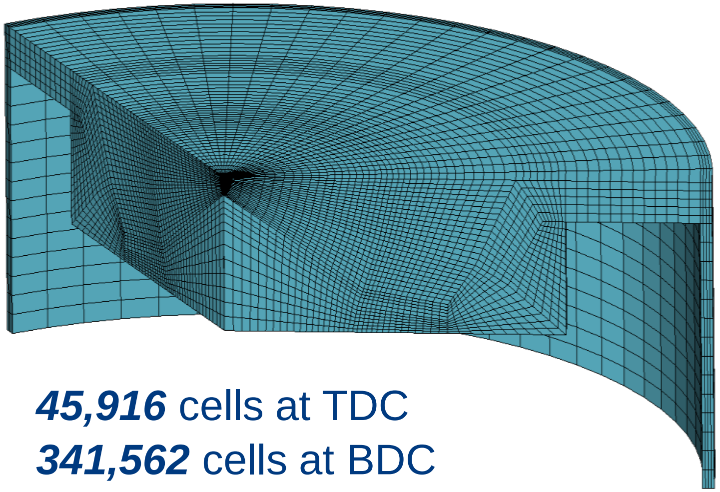
- Intensified Phantom v71
- Frame rate: 7.2kHz (1CAD)
- Exposure 55us
- Lens: 105mm UV f/4.5

Case Study: Light Duty Diesel Engine | ECN Spray B

Operating conditions:

Case name	900K	800K	1000K
Temperature at IVC [K]	380	340	454
Pressure at IVC [bar]	2.25	2.01	2.61
Temperature at TDC [K]	900	800	1000
Density at TDC [kg/m^3]		22.8	
Non-reacting O_2 [%]	7.5	-	-
Reacting O_2 [%]		15	
Injection pressure [bar]		1500	
Injected mass [mg/cycle]		3.68	
Engine Speed [rpm]		1200	
Inj. start [CAD ATDC]		-2.5	
Inj. duration [CAD]		11	

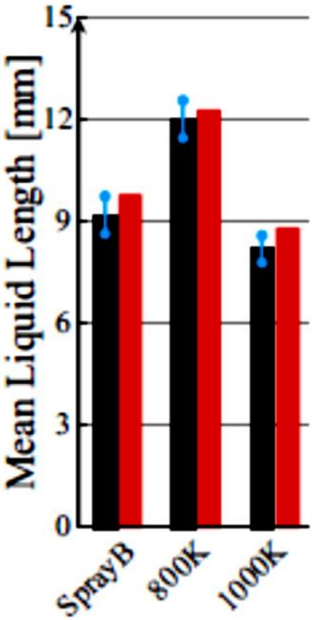
Spray oriented grid

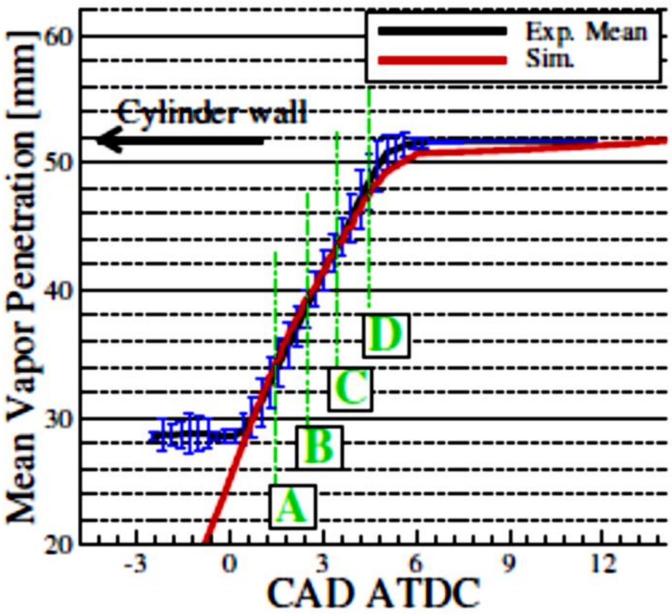


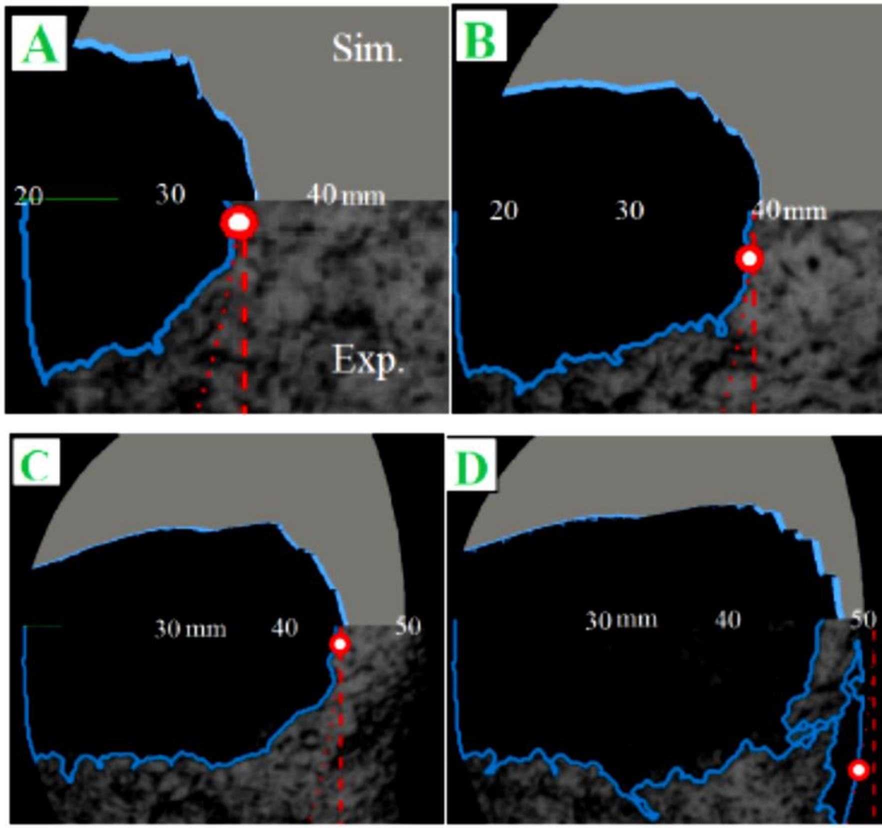
45,916 cells at TDC
341,562 cells at BDC
48.7 and ***11.2*** for maximum and average mesh non-orthogonality

Case Study: Light Duty Diesel Engine | ECN Spray B

Non-reacting: Liquid/vapor penetration

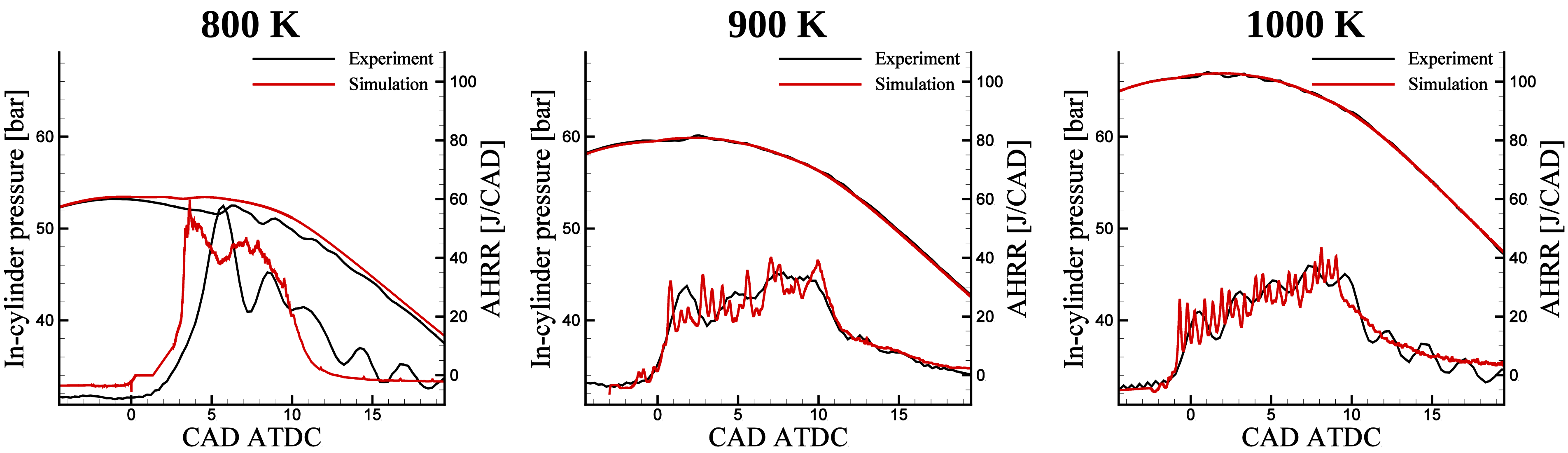






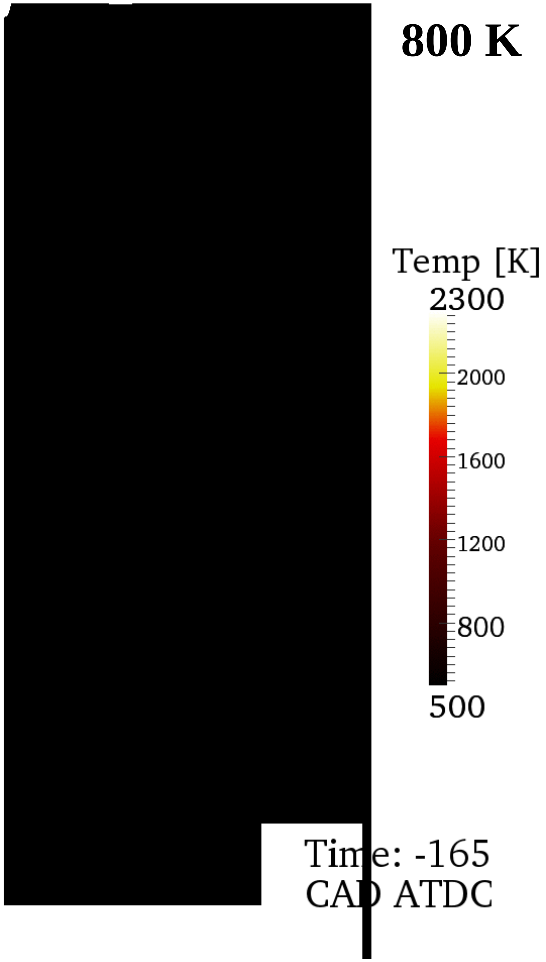
Case Study: Light Duty Diesel Engine | ECN Spray B

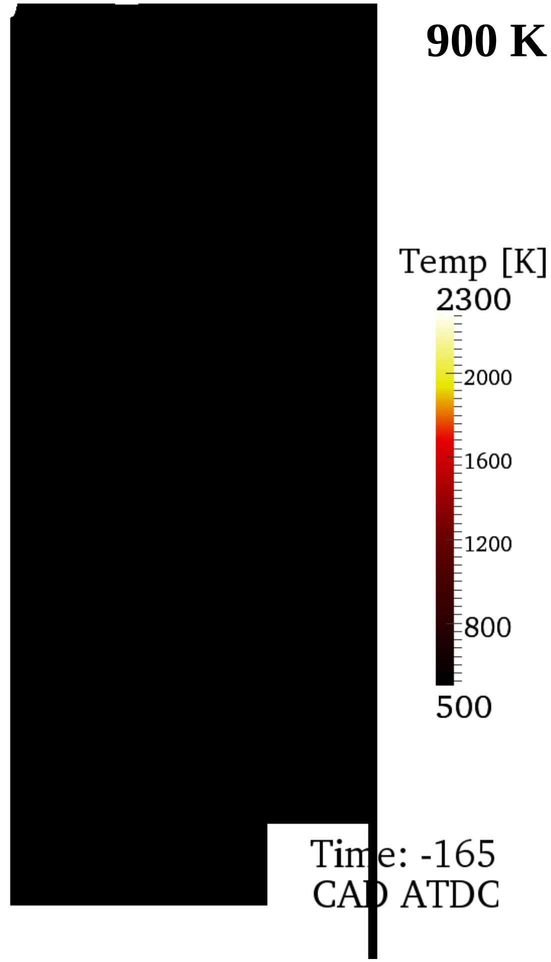
Reacting: In-cylinder Pressure and AHRR

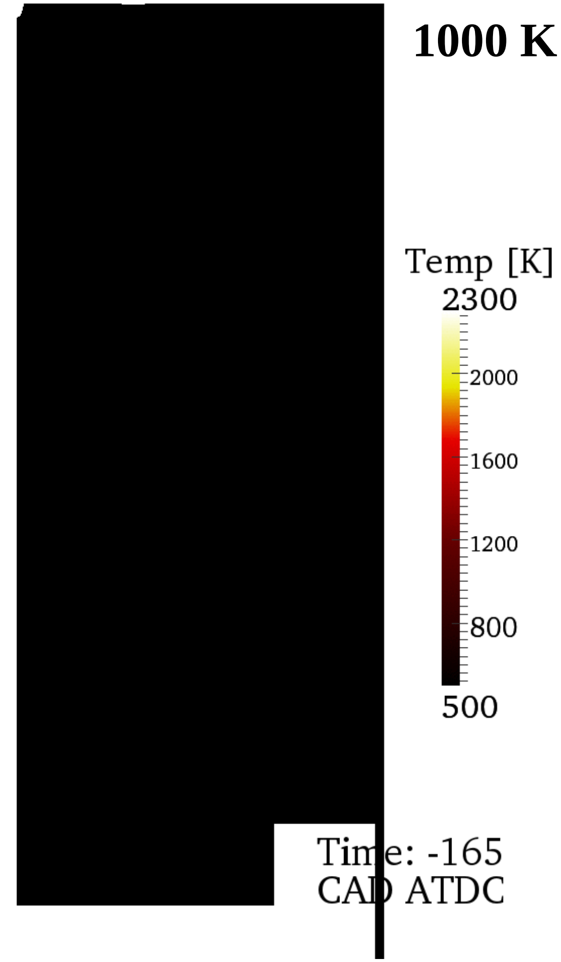


Case Study: Light Duty Diesel Engine | ECN Spray B

Reacting: Flame Lift-off

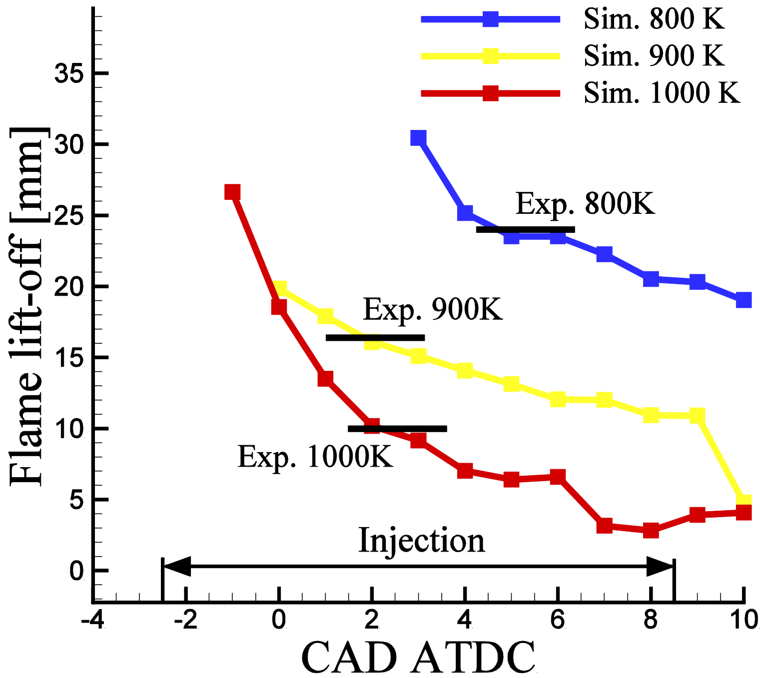


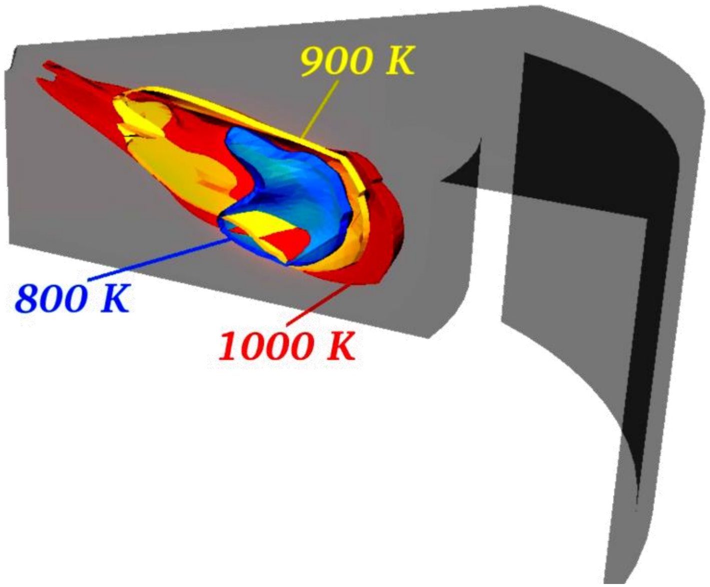




Case Study: Light Duty Diesel Engine | ECN Spray B

Reacting: Flame Lift-off





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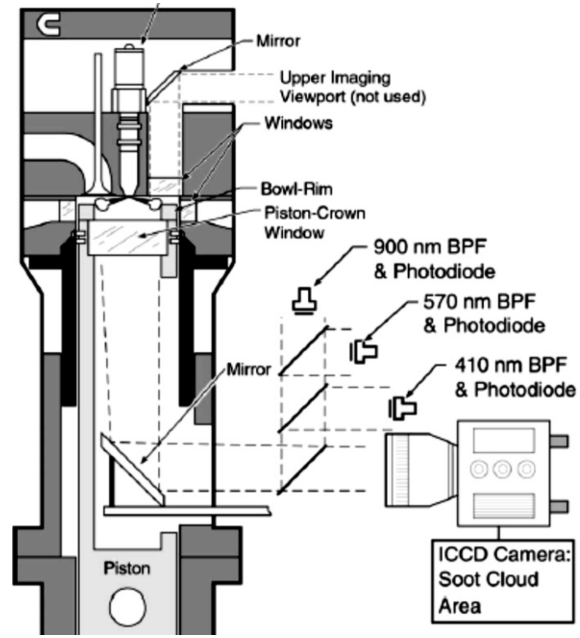
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Experimental configuration

SAE 2006-01-0055



Operating conditions

Case	HT-Sh-ID	HT-Lo-ID
Engine Speed [rpm]	1200	1200
Temperature at IVC [K]	384	320
Pressure at IVC [bar]	1.2	1.2
Temperature at TDC [K]	900	800
Density at TDC [kg/m^3]	24	22.3
Injected mass [mg/cycle]	61	61
Inj. start [CAD ATDC]	-7	-5
Inj. duration [CAD]	10	10
O_2 concentration [% by Vol.]	21	21

Number of cylinders	1
Number of intake valves	2
Number of exhaust valves	1*
Combustion chamber	Quiescent, direct injection
Swirl ratio	0.5
Bore × Stroke, cm	13.97 × 15.24
Bowl width, depth, cm	9.78, 1.55
Displacement, L	2.34
Connecting rod length, cm	30.48
Geometric compression ratio	11.2:1
Simulated compression ratio	16:1

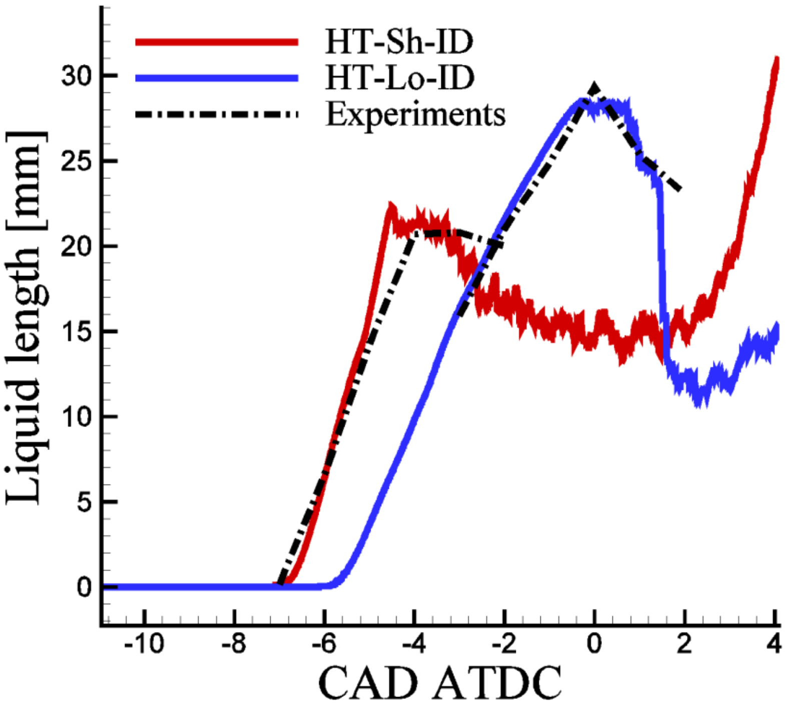
$$\text{Injected Mass}\Big|_{\text{Heavy Duty}} = 16.2 \times \text{Injected Mass}\Big|_{\text{Spray B}}$$

Case Study: Heavy Duty Diesel Engine | Sandia Engine

Non-reacting: Liquid penetration

Operating conditions

Case	HT-Sh-ID	HT-Lo-ID
Engine Speed [rpm]	1200	1200
Temperature at IVC [K]	384	320
Pressure at IVC [bar]	1.2	1.2
Temperature at TDC [K]	900	800
Density at TDC [kg/m^3]	24	22.3
Injected mass [mg/cycle]	61	61
Inj. start [CAD ATDC]	-7	-5
Inj. duration [CAD]	10	10
O_2 concentration [% by Vol.]	21	21



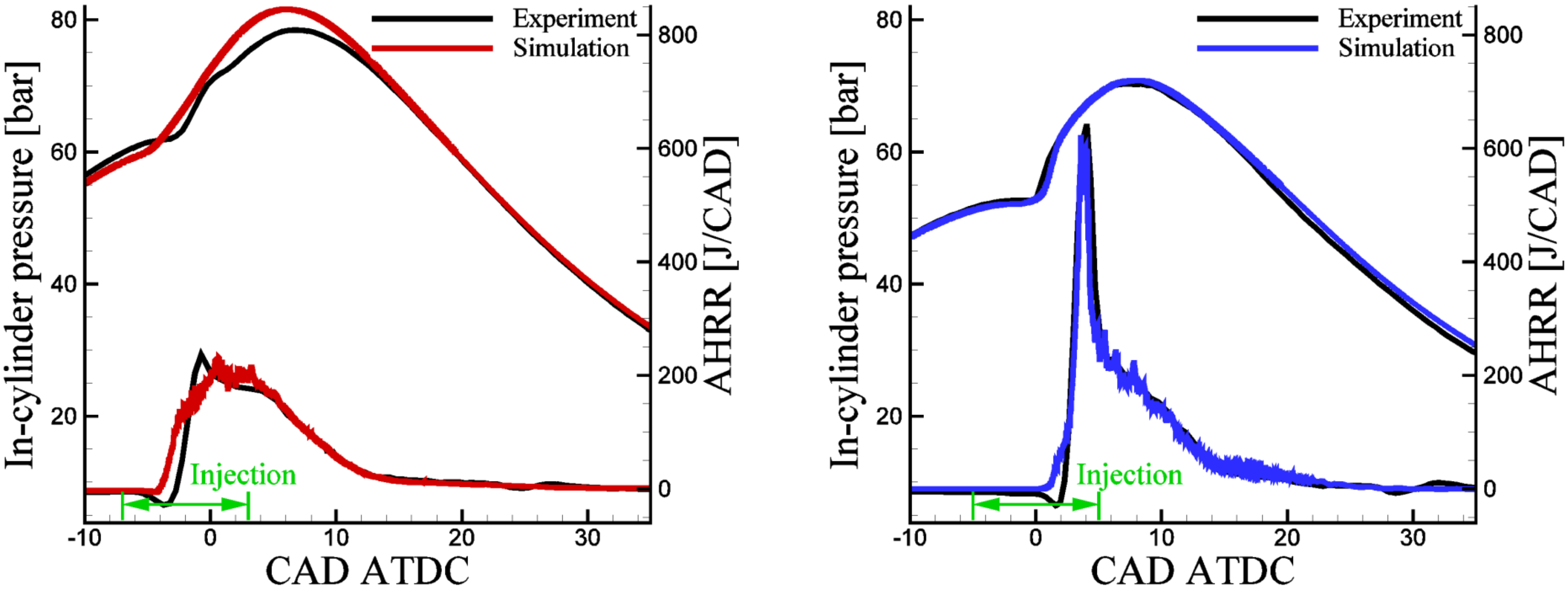
$$\text{Injected Mass}\Big|_{\text{Heavy Duty}} = 16.2 \times \text{Injected Mass}\Big|_{\text{Spray B}}$$

Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: In-cylinder Pressure & AHRR

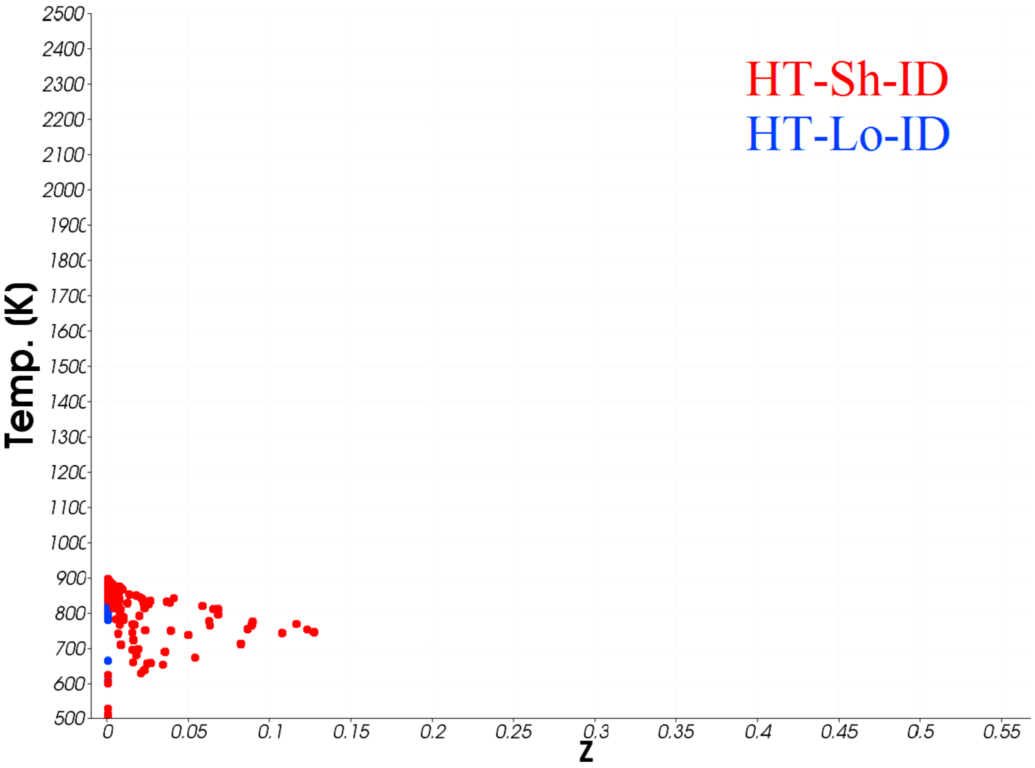
HT-Sh-ID

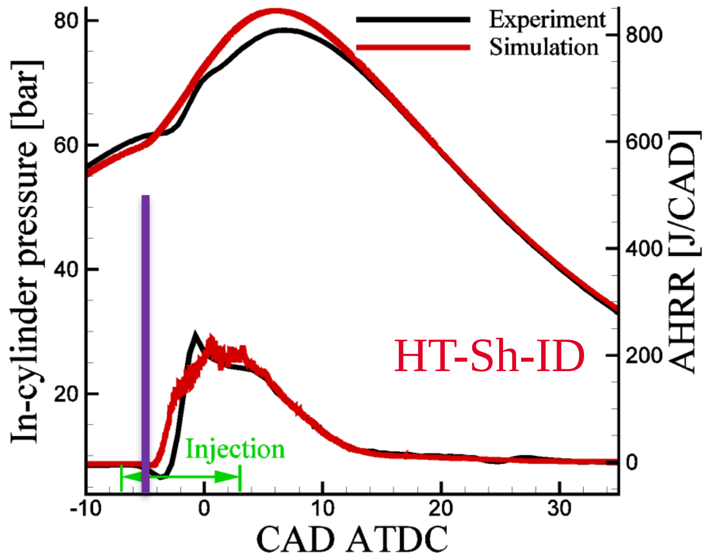
HT-Lo-ID

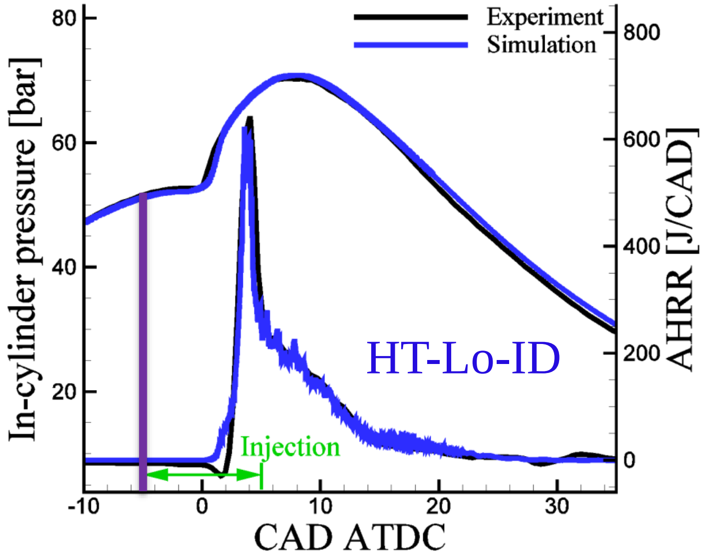


Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at -5 CAD ATDC

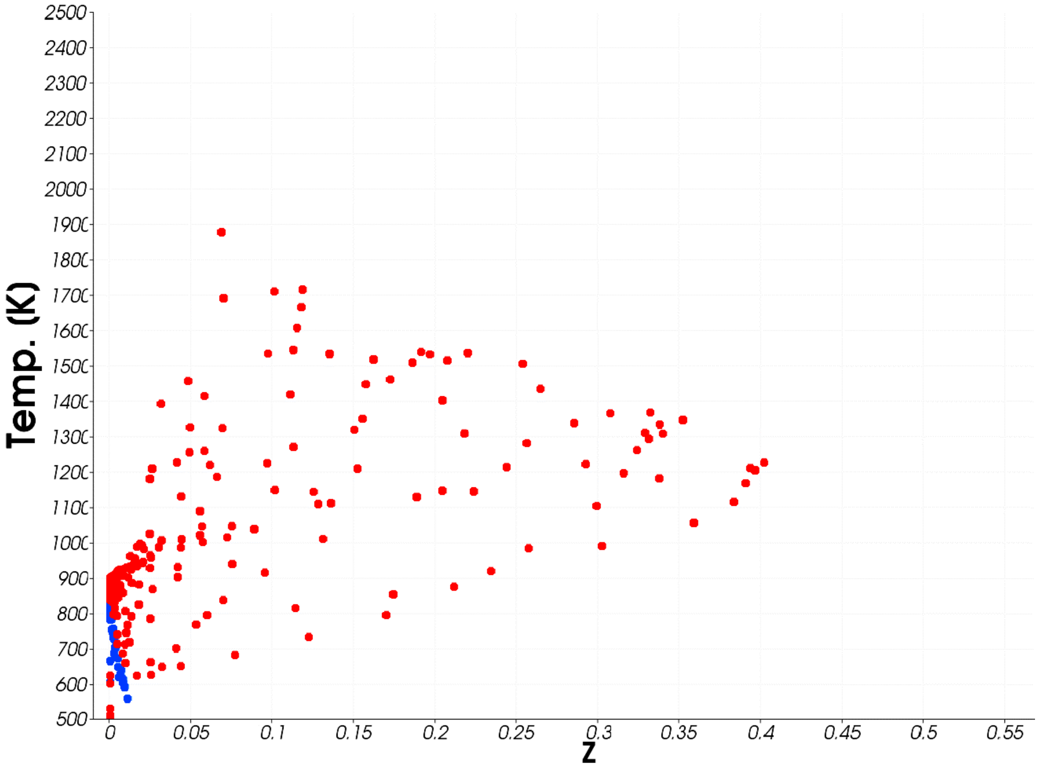


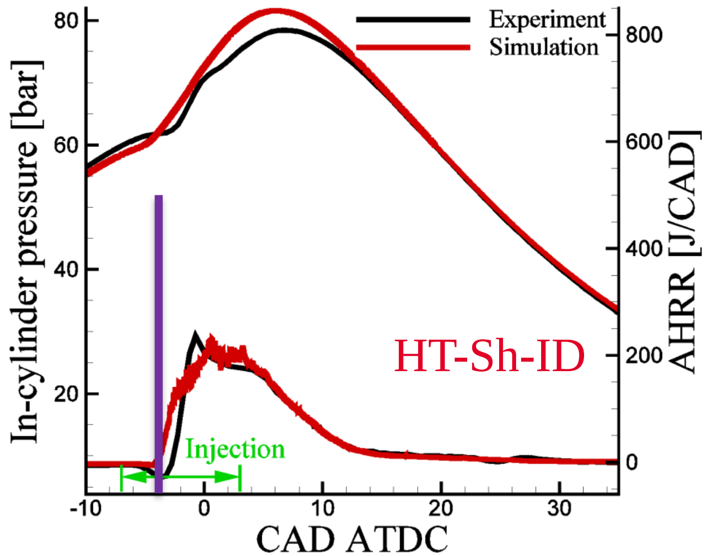


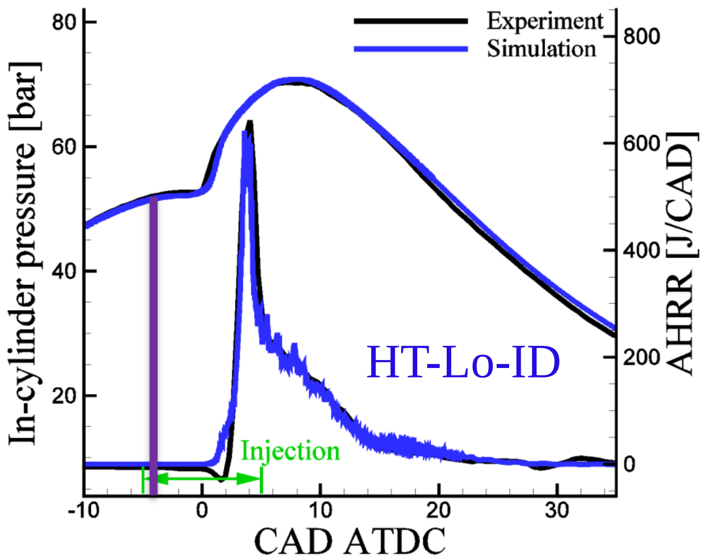


Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at -4 CAD ATDC

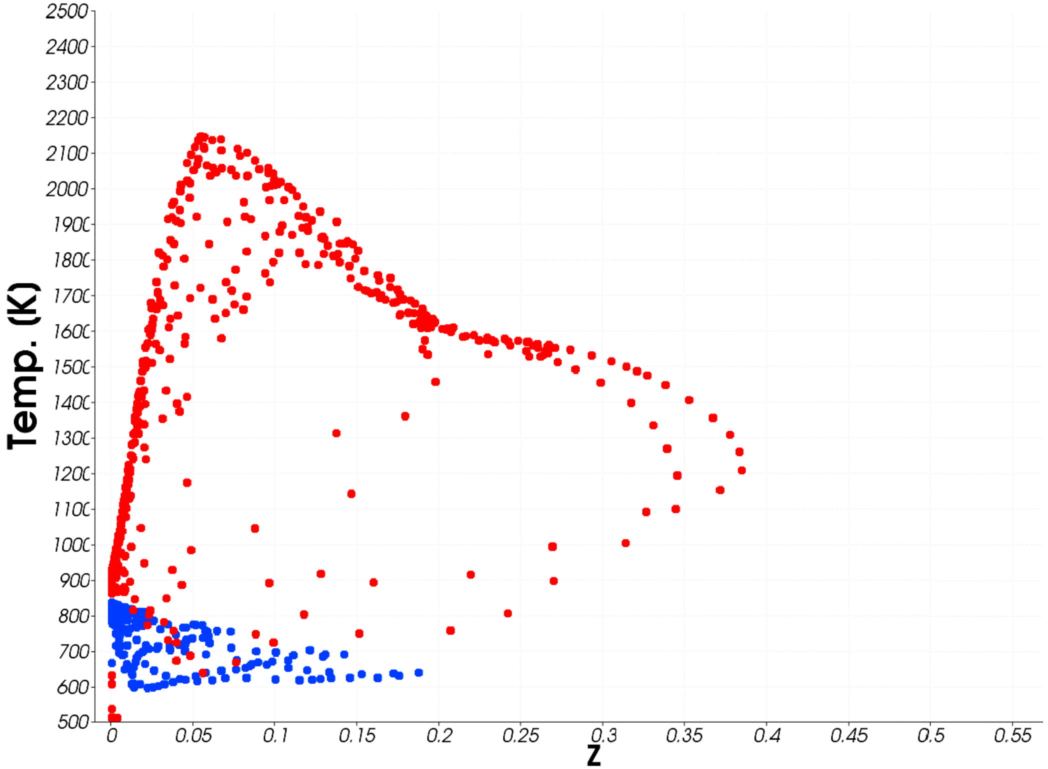


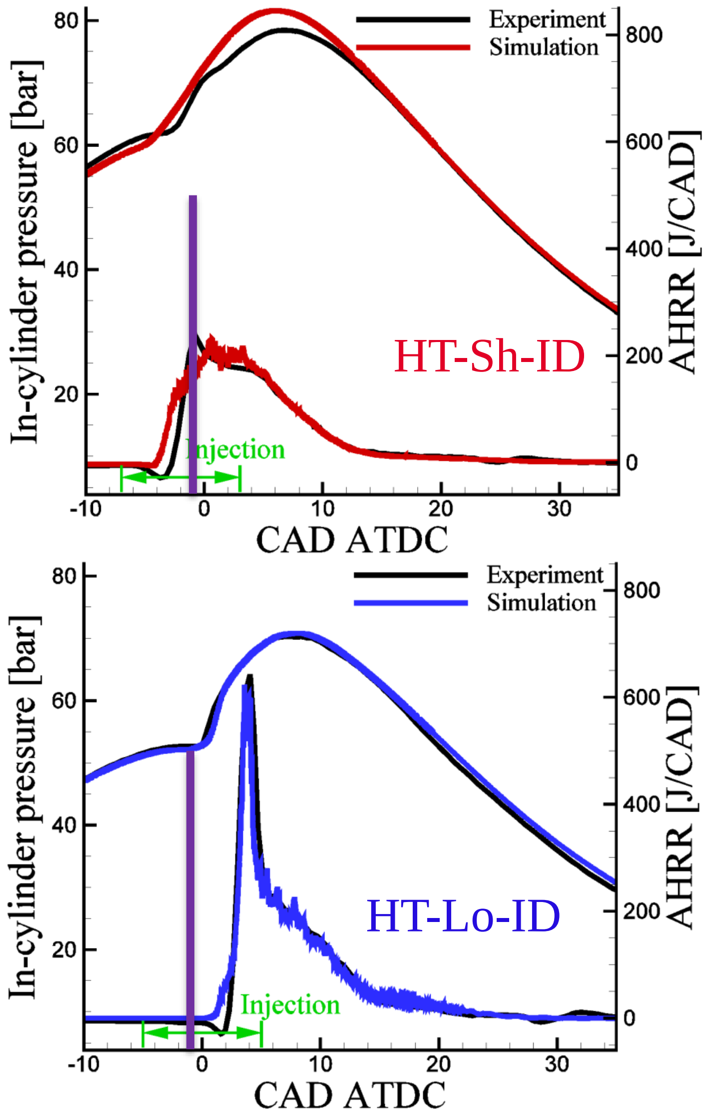




Case Study: Heavy Duty Diesel Engine | Sandia Engine

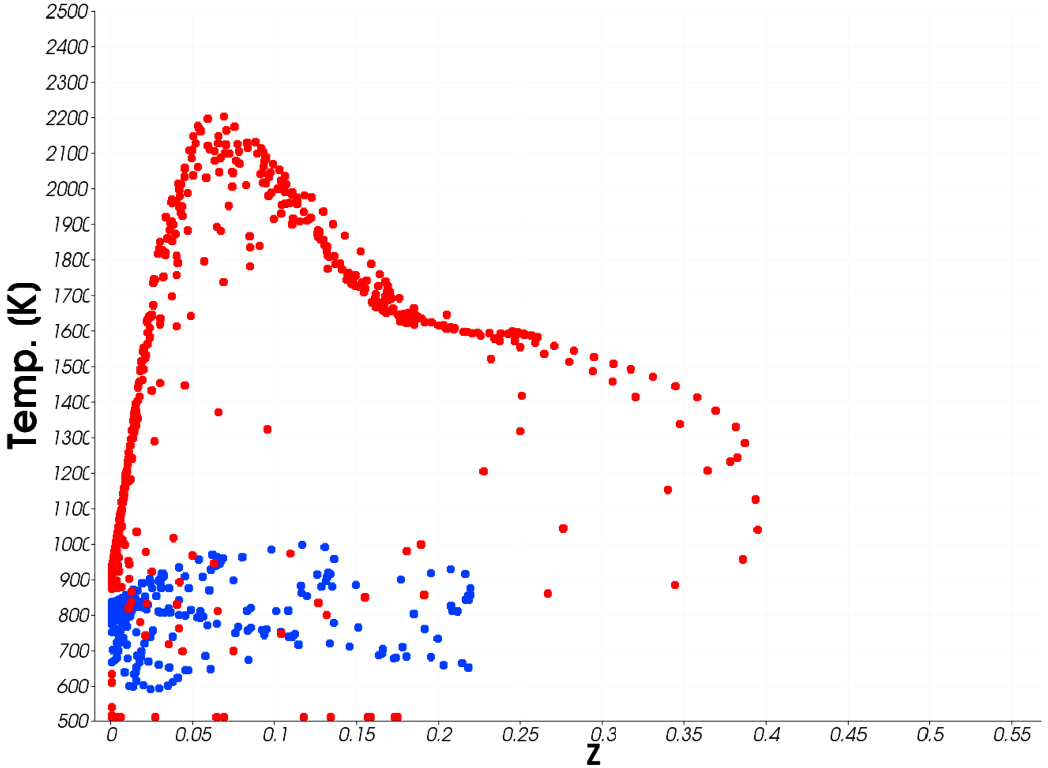
Reacting: Flame Structure at -1 CAD ATDC

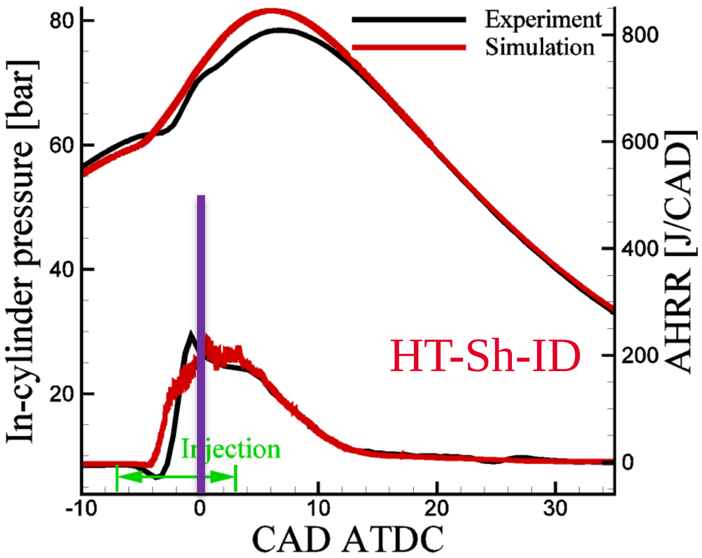


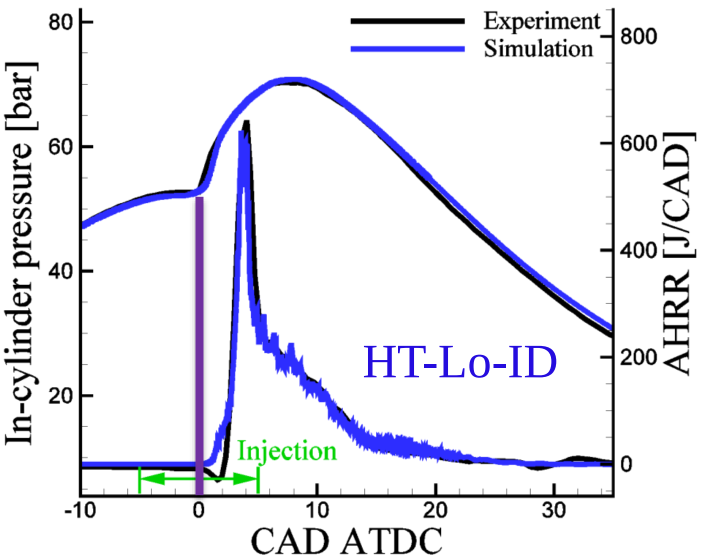


Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at TDC

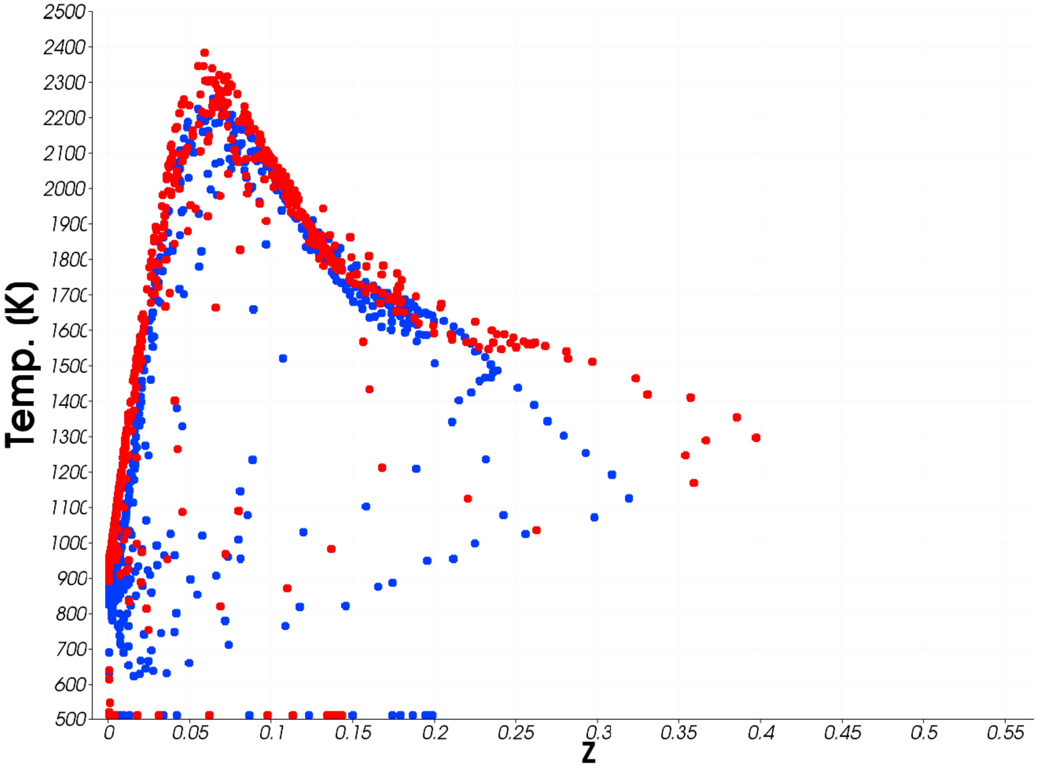


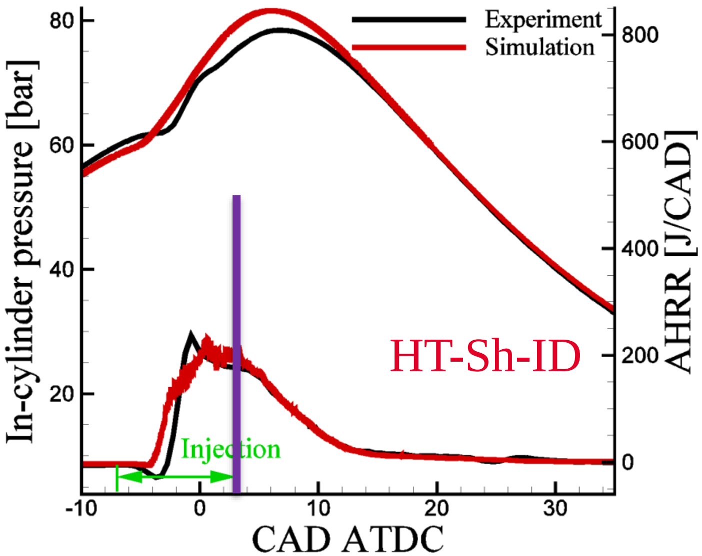


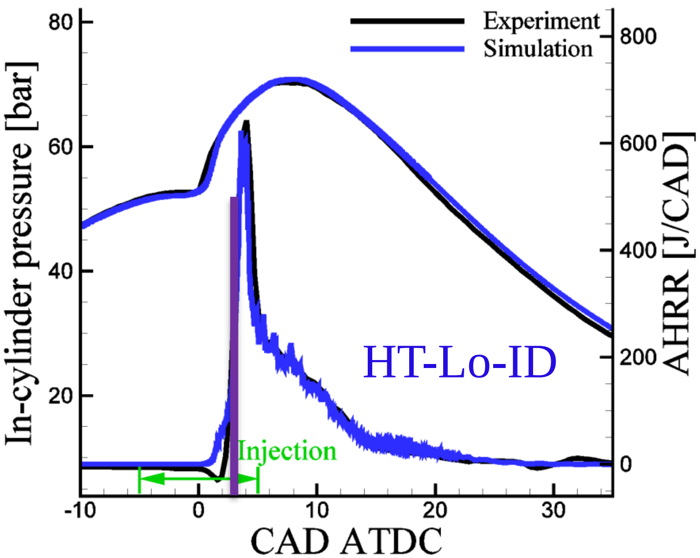


Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at 3 CAD ATDC







Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions

Conclusions

- ✓ FGM combustion closure was incorporated into OpenFOAM and Lib-ICE to model reacting spray and Diesel engine conditions.
- ✓ Progress variable source provided by FGM tabulation was capable of accurate predictions for state of thermodynamics of the mixture under non/partially premixed combustion configurations.
- ✓ For studied ambient temperature conditions, results of ignition delay, PRR or AHRR as well as flame lift-off was well agreeing with the experiments.
- ✓ n-dodecane chemical kinetics still suffers from comprehensive mechanism for low temperature combustion and there is a need for an extensively validated mechanism.

Thanks for your attention!

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