Third Two-Day Meeting on Internal Combustion Engine Simulations Using the OpenFOAM technology, Milan 22-23 February 2018.

Validation of combustion models with tabulated kinetics for compression ignition engines operating with advanced combustion modes

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Topics

Tabulated kinetics for combustion modeling in CI engines

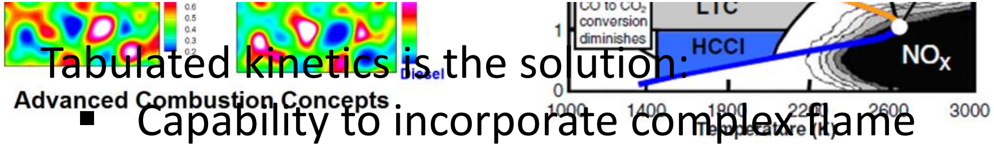
1) Motivation
2) Tabulation based on homogeneous reactor
3) Combustion models based on tabulated kinetics
   - Well-mixed model
   - Presumed PDF
   - RIF with tabulated kinetics
   - Flamelet progress variable
   - Dual-fuel combustion
4) Validation
   - Conventional Diesel
   - PCCI combustion
   - Dual-fuel combustion

Motivation

Why tabulated kinetics?

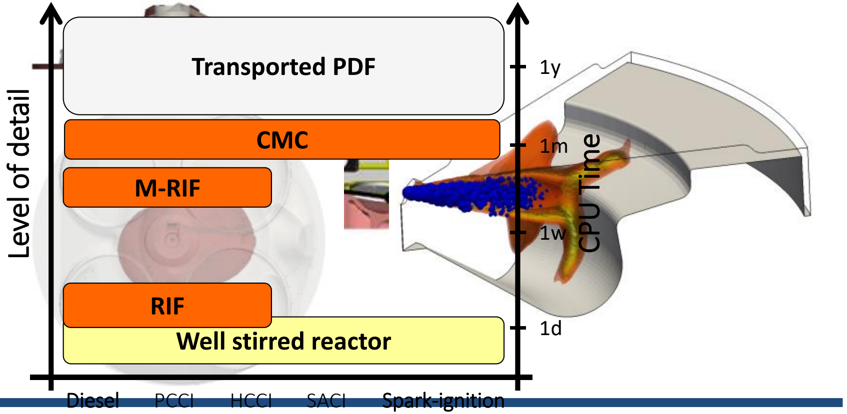
- New combustion modes and fuels to further reduce fuel consumption and pollutant emissions:
  - Dual fuel (Diesel-Natural gas, RCCI)
  - Single-fuel, kinetically controlled (PCCI, HCCI, spark-assisted)
  - New fuels (bio, carbon-neutral...)

- Virtualization of engine design:
  - CFD has a crucial role
  - Fast, accurate, robust models for prediction of engine performance and pollutant emissions
  - Need to find a compromise between:
    - Computational efficiency
    - Complex flame structures and kinetic schemes



Advanced Combustion Concepts

- Tabulated kinetics is the solution:
  - Capability to incorporate complex flame structures and kinetics schemes
  - Reduced CPU time

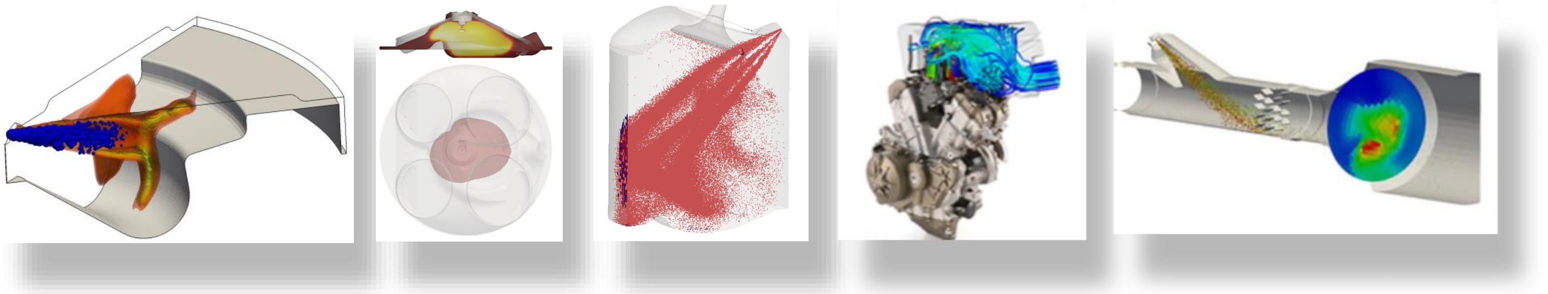


Lib-ICE

Internal combustion engine modeling using the OpenFOAM® technology

- Mesh motion for complex geometries
- Combustion
- Lagrangian sprays + liquid film
- Unsteady flows in intake and exhaust systems: plenums, silencers, 1D-3D coupling.
- Reacting flows in after-treatment devices: DPF, catalyst, SCR.

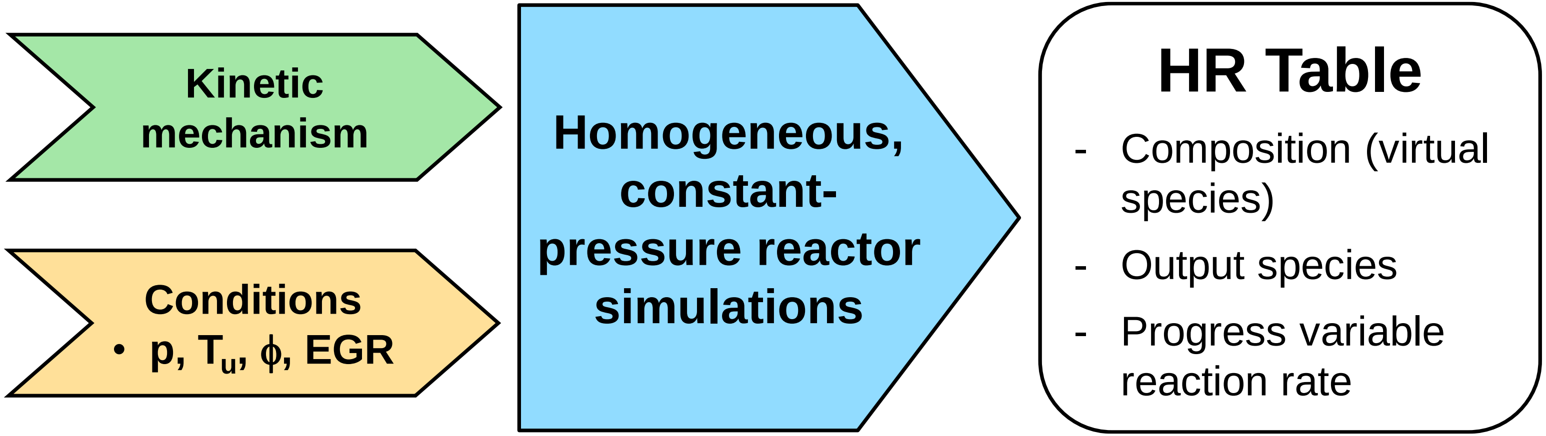
Lib ICE



Tabulated kinetics

Tabulated kinetics

Constant-pressure homogeneous reactor tabulation



Kinetic mechanism

Conditions
- **p, T_u, ϕ, EGR**

Homogeneous, constant-pressure reactor simulations

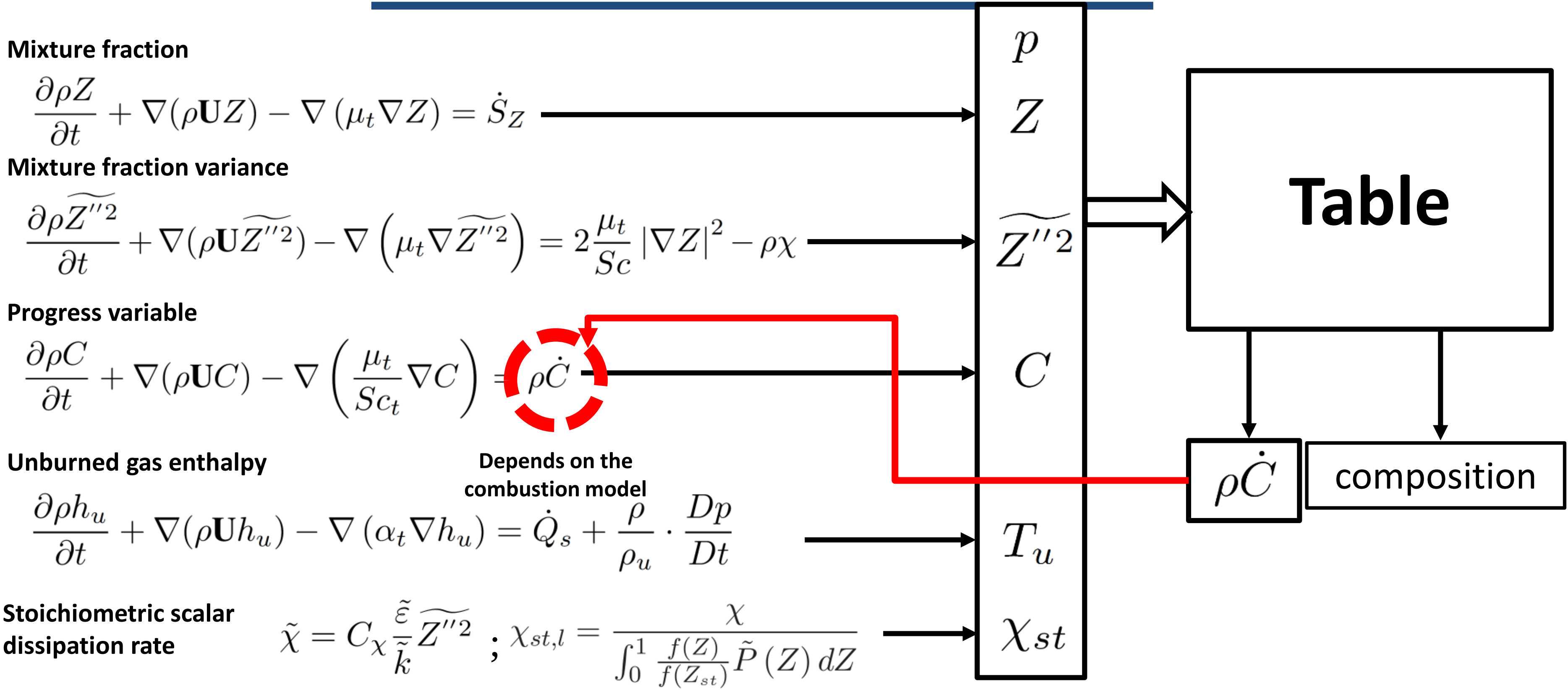
HR Table
- Composition (virtual species)
- Output species
- Progress variable reaction rate

The table generator is PYTHON script using the CANTERA library:
- highly flexible
- fast, reliable
- fully parallel

Acknowledgment: MSc Student Alberto Comolli

Tabulated kinetics

Governing equations



Mixture fraction

$$\frac{\partial \rho Z}{\partial t} + \nabla(\rho \mathbf{U} Z) - \nabla\left(\mu_t \nabla Z\right) = \dot{S}_Z$$

Mixture fraction variance

$$\frac{\partial \rho \widetilde{Z''^2}}{\partial t} + \nabla(\rho \mathbf{U} \widetilde{Z''^2}) - \nabla\left(\mu_t \nabla \widetilde{Z''^2}\right) = 2\frac{\mu_t}{Sc}\left|\nabla Z\right|^2 - \rho\chi$$

Progress variable

$$\frac{\partial \rho C}{\partial t} + \nabla(\rho \mathbf{U} C) - \nabla\left(\frac{\mu_t}{Sc_t}\nabla C\right) = \rho\dot{C}$$

Depends on the combustion model

Unburned gas enthalpy

$$\frac{\partial \rho h_u}{\partial t} + \nabla(\rho \mathbf{U} h_u) - \nabla\left(\alpha_t \nabla h_u\right) = \dot{Q}_s + \frac{\rho}{\rho_u}\cdot\frac{Dp}{Dt}$$

Stoichiometric scalar dissipation rate

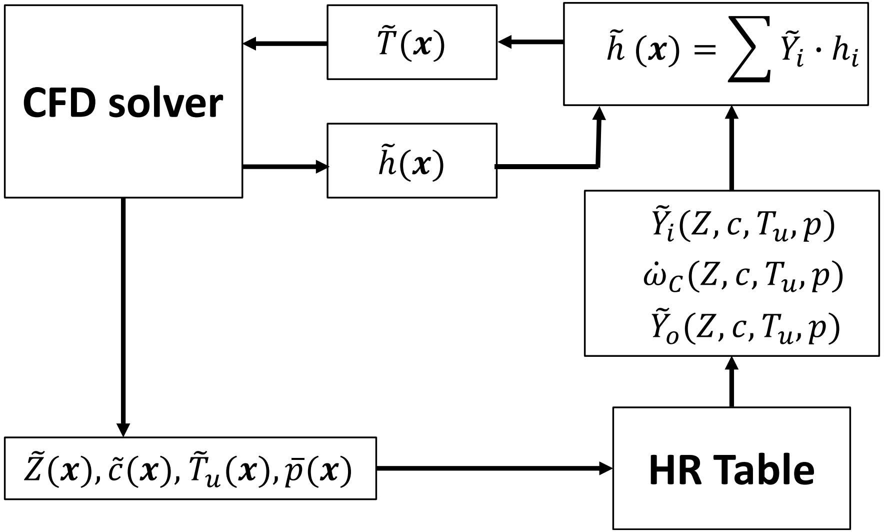
$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{Z''^2} \; ; \; \chi_{st,l} = \frac{\chi}{\int_0^1 \frac{f(Z)}{f(Z_{st})}\tilde{P}(Z)\,dZ}$$

Tabulated kinetics

Combustion models

TWM: tabulated well-mixed

- **No turbulence-chemistry interaction**



CFD solver

$\tilde{T}(\boldsymbol{x})$

$\tilde{h}\,(\boldsymbol{x}) = \sum \tilde{Y}_i \cdot h_i$

$\tilde{h}(\boldsymbol{x})$

$\tilde{Y}_i(Z,c,T_u,p)$

$\dot{\omega}_C(Z,c,T_u,p)$

$\tilde{Y}_o(Z,c,T_u,p)$

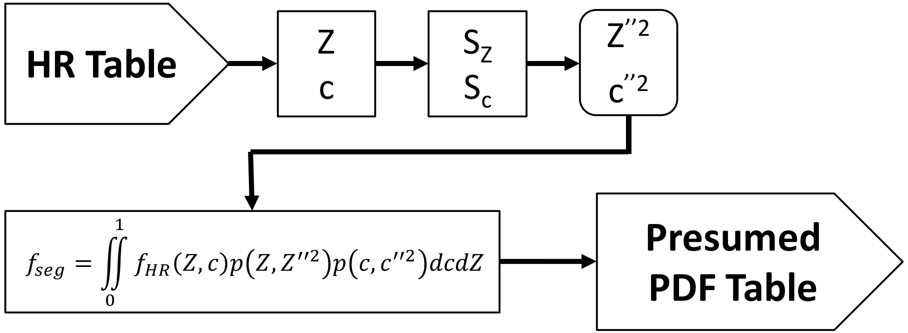
$\tilde{Z}(\boldsymbol{x}), \tilde{c}(\boldsymbol{x}), \tilde{T}_u(\boldsymbol{x}), \bar{p}(\boldsymbol{x})$

HR Table

TPPDF: tabulated presumed PDF

$$\dot{C} = \iint_0^1 \dot{C}(Z,c)\beta\left(Z,Z''^2\right)\delta\left(c,c''^2\right)dcdZ$$

- **Only fluctuations, no sub-grid mixing**
- HR Table is processed to include the effects of mixture fraction fluctuations in the calculation of the PV source term and composition.



HR Table

Z
c

S_Z
S_c

Z''^2
c''^2

$f_{seg} = \iint_0^1 f_{HR}(Z,c)p\left(Z,Z''^2\right)p\left(c,c''^2\right)dcdZ$

Presumed PDF Table

Tabulated kinetics

Combustion models

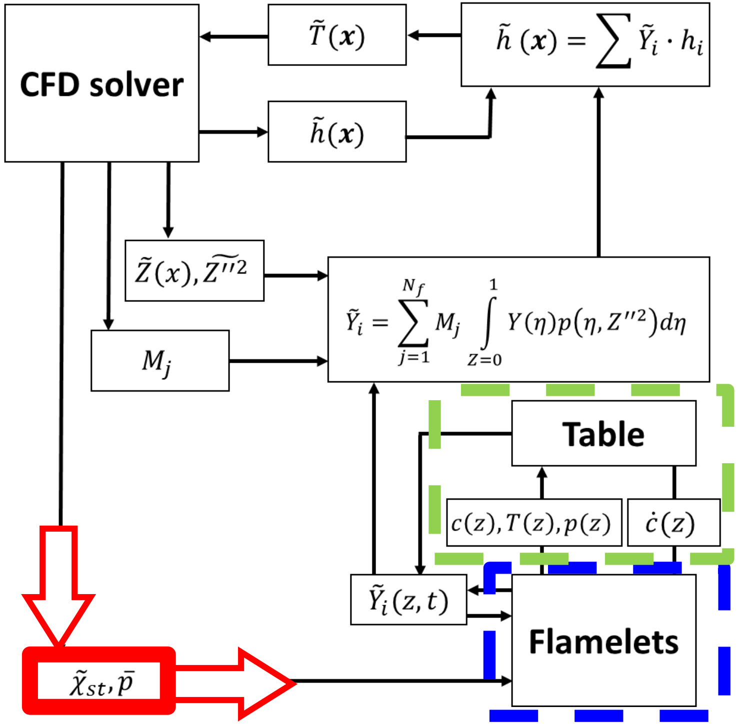
Tabulated Representative Interactive Flamelet (TRIF)

- Laminar flamelet concept applied to describe Diesel combustion.
- Flamelet equations are solved in the Z-domain using tabulated kinetics

$$\frac{\partial C}{\partial t} = \frac{\chi_Z}{2}\frac{\partial^2 C}{\partial Z^2} + \dot{C}$$

$$\frac{\partial h}{\partial t} = \frac{\chi_Z}{2}\frac{\partial^2 h}{\partial Z^2} + \frac{1}{\rho}\frac{dp}{dt}$$

- The rest of the model is like the standard RIF:
  - On-line beta-PDF integration
  - Possibility to use multiple flamelets

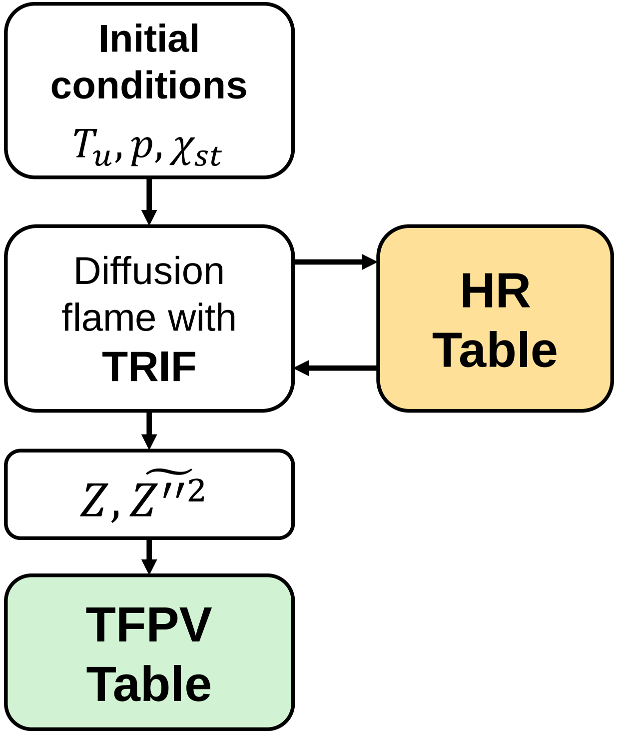


Tabulated kinetics

Combustion models

Tabulated flamelet progress variable TFPV

- Approach similar to ADF (Approximated Diffusion Flames)
- Turbulence/chemistry interaction, sub-grid mixing and premixed flame propagation.
- Progress variable reaction rate function also of the stoichiometric scalar dissipation rate χ_{st}
- Correct estimation of
  - extinction in the near nozzle region;
  - re-ignition;
  - flame stabilization process;
- TFPV table generated using TRIF and a variable time-step strategy to reduce the required computational time.



Tabulated kinetics

Combustion models: dual fuel combustion

Assumptions

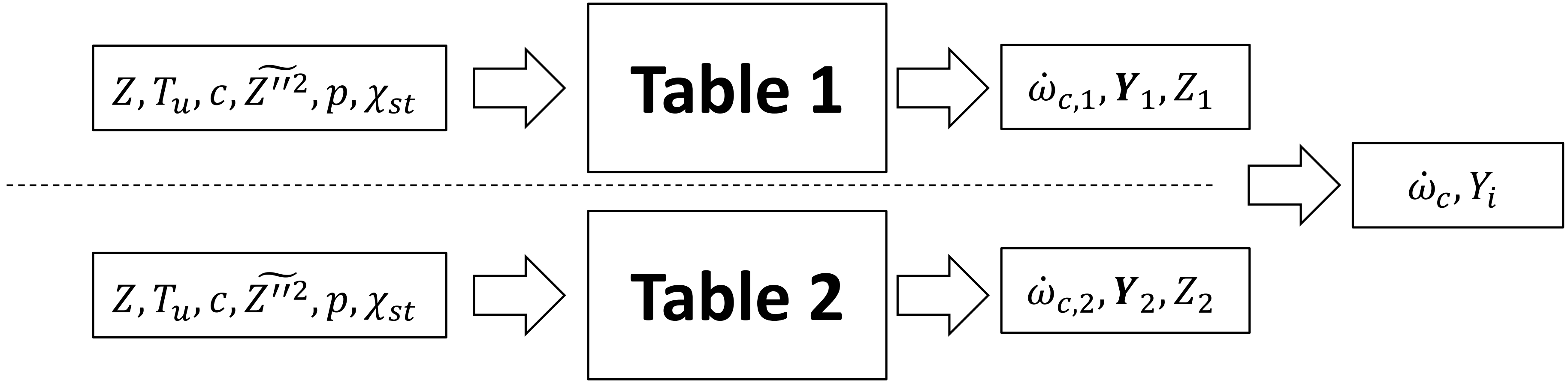
- One progress variable in any cell
- Ignition governed by progress variable diffusion and local conditions (pressure, temperature, mixture fraction)
  - One table for any fuel
- Homogeneous mixture
  - Air is uniformily distributed among the two fuels ("single fuel mixture fraction" is equal to the global mixture fraction)

Model

- Transport equations for the two fuel mixture fractions (Z_1 and Z_2)
- Progress variable reaction rate is computed as the weighted average of the corresponding values for the two fuels.

Tabulated kinetics

Combustion models: dual fuel combustion



$Z, T_u, c, \widetilde{Z''^2}, p, \chi_{st}$

Table 1

$\dot{\omega}_{c,1}, \boldsymbol{Y}_1, Z_1$

$Z, T_u, c, \widetilde{Z''^2}, p, \chi_{st}$

Table 2

$\dot{\omega}_{c,2}, \boldsymbol{Y}_2, Z_2$

$\dot{\omega}_c, Y_i$

Progress variable source term

$$\dot{\omega}_c = \frac{Z_1 \cdot \dot{\omega}_{c,1}\left(T_u, Z, \widetilde{Z''^2}, p, c\right) + Z_2 \cdot \dot{\omega}_{c,2}\left(T_u, Z, \widetilde{Z''^2}, p, c\right)}{Z_1 + Z_2}$$

Composition

$$\boldsymbol{Y} = \frac{Z_1 \cdot \boldsymbol{Y}_1\left(T_u, Z, \widetilde{Z''^2}, p, c\right) + Z_2 \cdot \boldsymbol{Y}_2\left(T_u, Z, \widetilde{Z''^2}, p, c\right)}{Z_1 + Z_2}$$

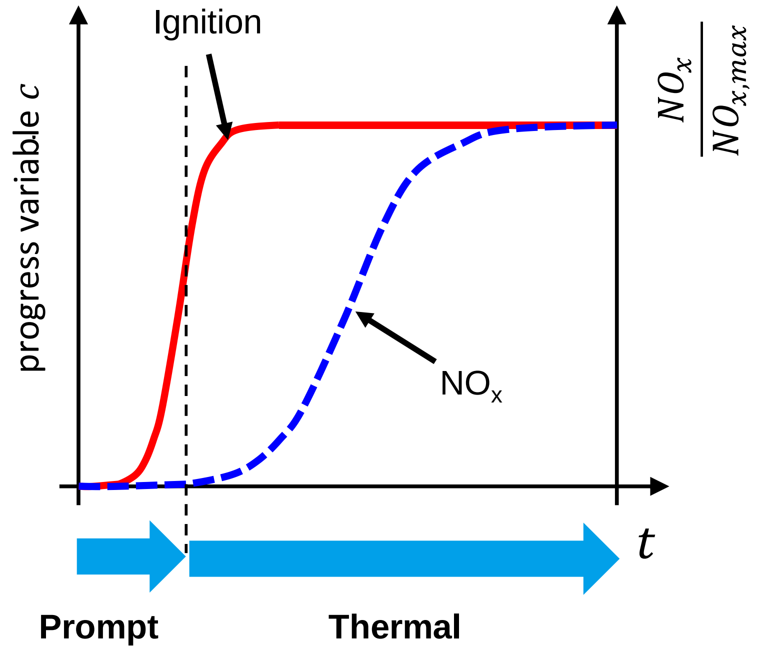
Pollutant emissions

Tabulated NO$_x$

- NO$_x$ progress variable:
  - ➢ $c_{NO_x} = \frac{Y_{NO_x}}{Y_{NO_x,eq}}$
  - ➢ $Y_{NO_x} = Y_{NO} + Y_{NO_2} + Y_{N_2O} + Y_{N_2O_2}$
- NO$_x$ formation and ignition have different time scales

$$\frac{\partial \bar{\rho} \tilde{Y}_{NO_x}}{\partial t} + \nabla \cdot \left(\bar{\rho} \tilde{\mathbf{U}} \tilde{Y}_{NO_x} \right) - \nabla \cdot \left(\frac{\tilde{\mu}_t}{Sc_t} \nabla \tilde{Y}_{NO_x} \right) = \dot{\omega}_{NO_x}$$

- ▪ A combustion progress variable threshold value is used to select the expression for $\dot{\omega}_{NO_x}$
  - ➢ c < 0.5 : $\dot{\omega}_{NO_x} = \dot{\omega}_{NO_x}(C)$
  - ➢ c > 0.5 : $\dot{\omega}_{NO_x} = \dot{\omega}_{NO_x}(C_{NO_x})$



Pollutant emissions

Soot

- Leung, Lindsted and Jones Model. Two transport equations solved for particle number density N_p and soot volume fraction f_v accounting for inception, coagulation, surface growth and oxidation:

$$\dot{\omega}_{N_p} = \dot{\omega}_{inception} - \dot{\omega}_{coagulation}$$

$$\dot{\omega}_{f_v} = \dot{\omega}_{inception} + \dot{\omega}_{surface\ growth} - \dot{\omega}_{oxi\ O_2} - \dot{\omega}_{oxi\ OH}$$

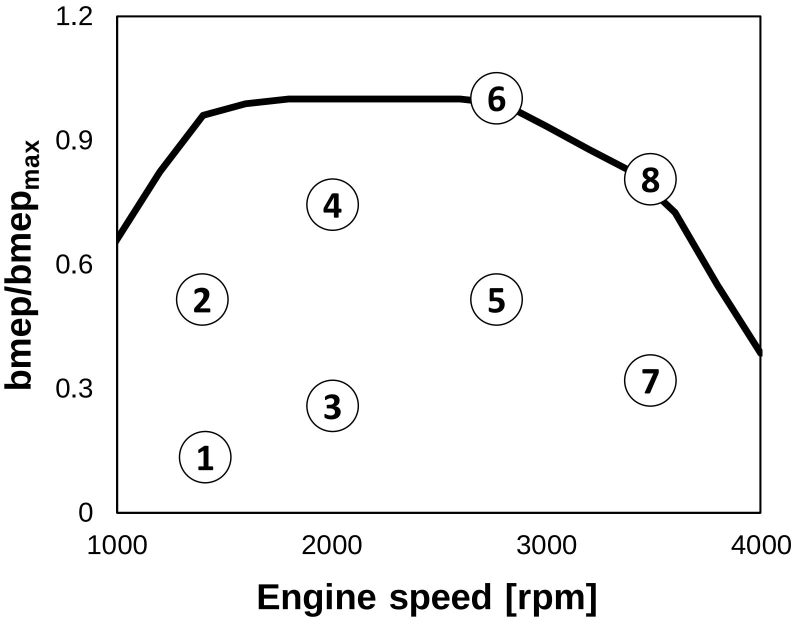
➢ Acetylene (C_2H_2) used as soot precursor species, inception and surface growth quantities computed using the averaged acetylene concentration in each computational cell.

Validation

Validation: FPT F1C Engine

Conventional Diesel

Selected operating points



Bore	96 mm
Stroke	104 mm
Compression ratio	18
IVC	-145 deg
EVO	110 deg

Swirl ratio	1.3
# holes	8
Nozzle hole diameter	140 μm
Homologation	**EU6**

	Name	[rpm]	load	λ	EGR	#inj
1	**HEGR**	1400	12%	2.7	40%	3
2	**1400x50**	1400	50%	1.4	15%	3
3	**A25**	2000	25%	2.1	20%	3
4	**A75**	2000	75%	1.3	15%	3
5	**B50**	2750	50%	1.4	15%	3
6	**B100**	2750	100%	1.3	5%	2
7	**C40**	3500	40%	2.3	10%	3
8	**C100**	3500	100%	1.5	0%	1

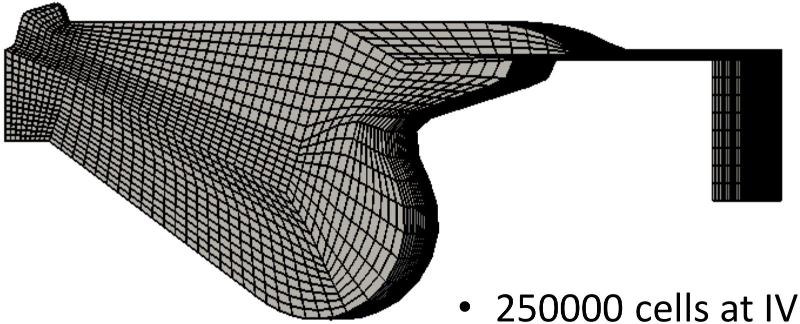
Validation: FPT F1C Engine

Conventional Diesel

Simulation setup

Mesh

- 1/8 of the combustion chamber, spray-oriented, automatically generated with the Python Polimi pre-processor



- 250000 cells at IVC
- 40000 cells at TDC

Tabulation

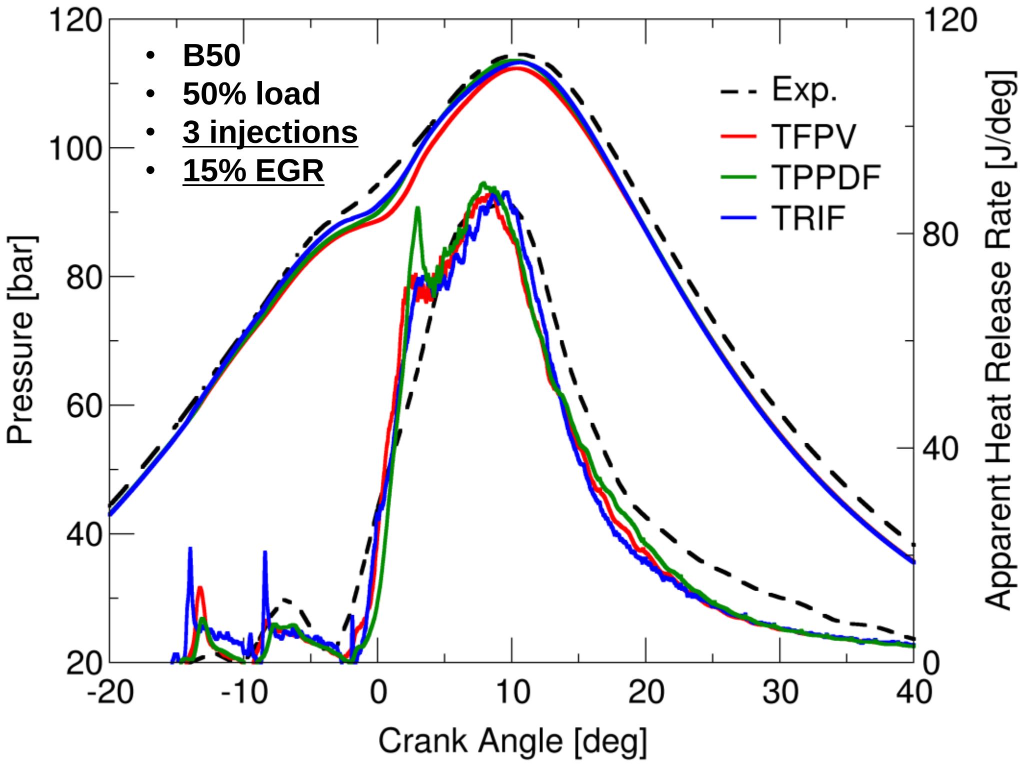
- **Fuel: n-$C_{12}H_{26}$**
- **Mechanism: Frassoldati et al (96 species)**

Temperature [K]	600 - 1300 K (step 50 K)
Pressure [bar]	20-200 (step 40)
Equivalence ratio	0-3 (finer resolution close to $\phi = 1$)
Mixture fraction segregation	0.0, 0.001 0.0025, 0.01, 0.025, 0.1 1.0
Scalar dissipation rate χ_{st} [1/s]	0, 1, 3, 7, 20, 55

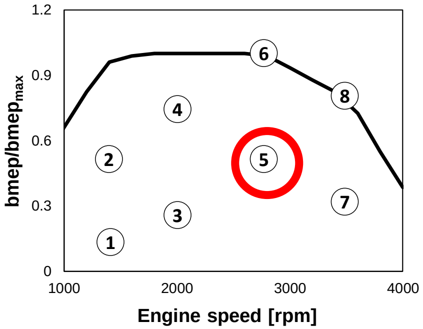
- **TPPDF, TRIF, TFPV models**

Validation: FPT F1C Engine

Conventional Diesel



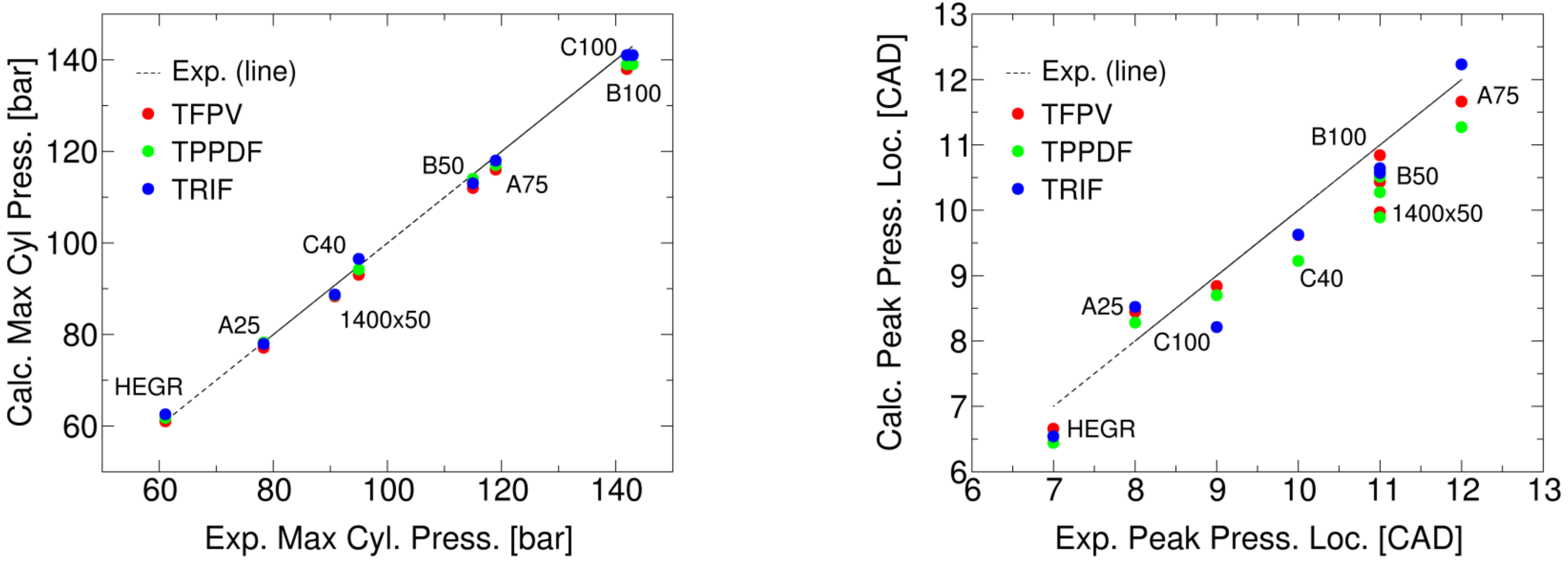
- **B50**
- **50% load**
- **<u>3 injections</u>**
- **<u>15% EGR</u>**



- Similar heat release rate during main combustion
- **Ignition delay:**
  - ⇨ TFPV ignites earlier than TRIF and TPPF during second and main injection events.

Validation: FPT F1C Engine

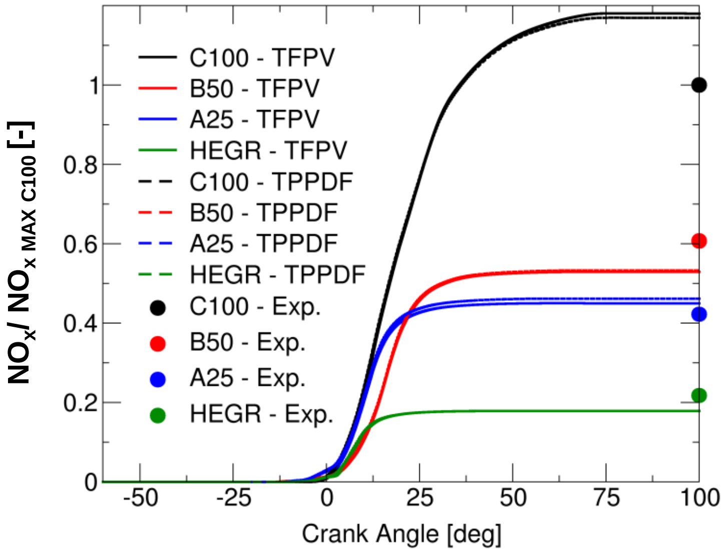
Conventional Diesel

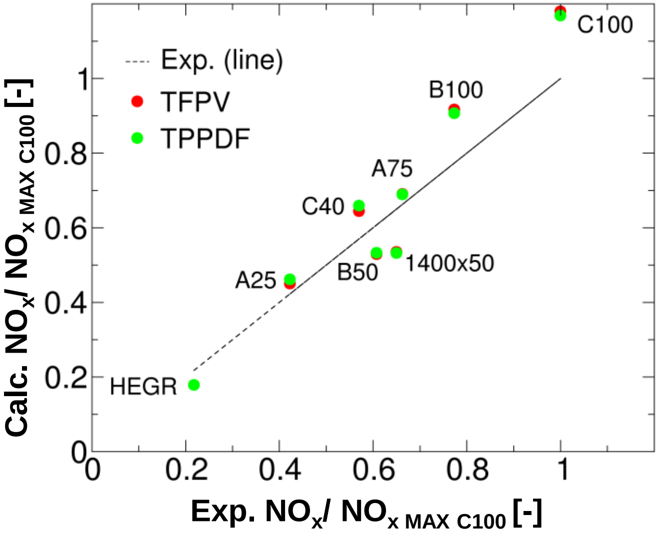


- All the models are able to capture in-cylinder pressure peak and its location
- CPU time: 15 hours on a 8 core machine for a power-cycle (dual-core, eight processor Intel Xeon E5-2630 v3 2.40GHz)

Validation: FPT F1C Engine

Conventional Diesel



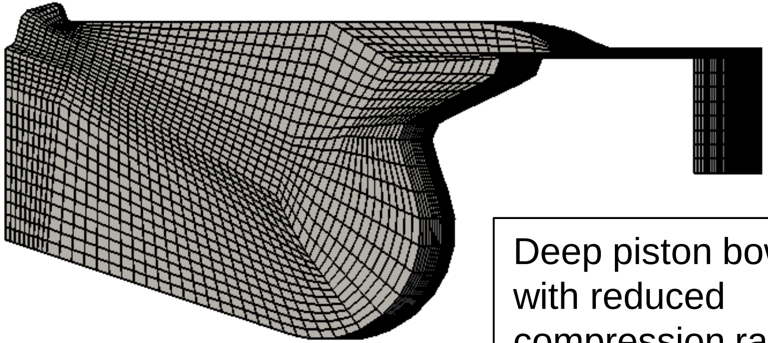


- NO_x grow during combustion procress and they are frozen when cylinder temperature decreases.
- All predictions fall in the ±20% range compared to experimental data.

Validation: FPT F1C Engine

PCCI combustion

Combustion chamber



Deep piston bowl with reduced compression ratio

Operating conditions

	Name	Speed [rpm]	bmep [bar]	λ	EGR
1	PCCI1	2000	5	~1.2	~40%
2	PCCI2	2000	7.5	~1.2	~40%
3	PCCI3	3000	5	~1.2	~40%

- Combustion model: TWM (TCI effects can be reasonably neglected)
- Fuel is n-heptane ($n\text{-}C_7H_{16}$) having similar CN as Diesel
- Tabulated mechanism: 159 species from LLNL

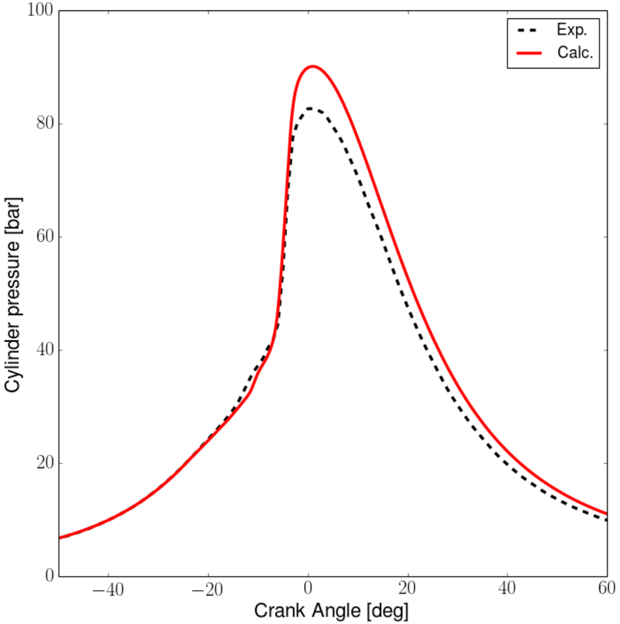
Table discretization

Temperature [K]	600-800 (step 25 K) 800 - 1000 (step 12.5 K) 1000 - 1100 (step 25 K) 1100 - 1200 (step 50 K)
Pressure [bar]	20-200 (step 20 bar)

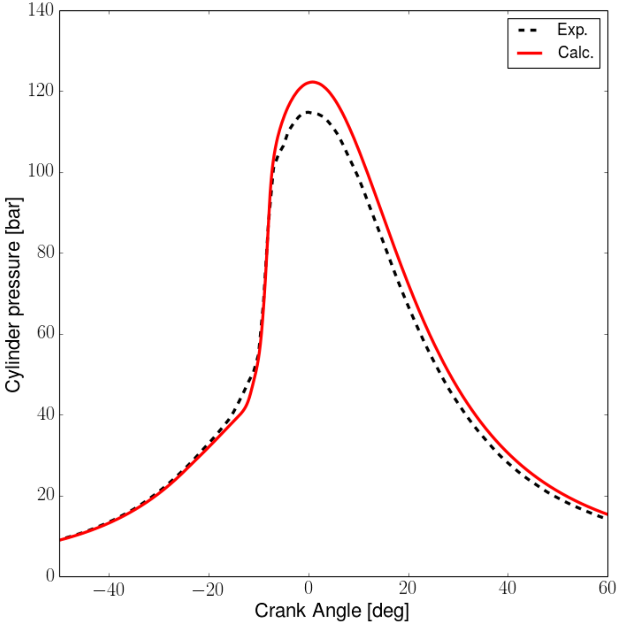
Validation: FPT F1C Engine

PCCI combustion: cylinder pressure

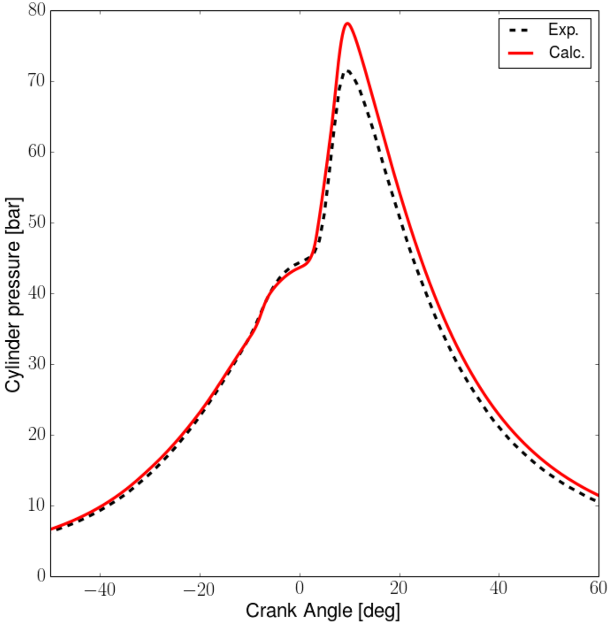
PCCI1: 2000x5



PCCI2: 2000x7.5



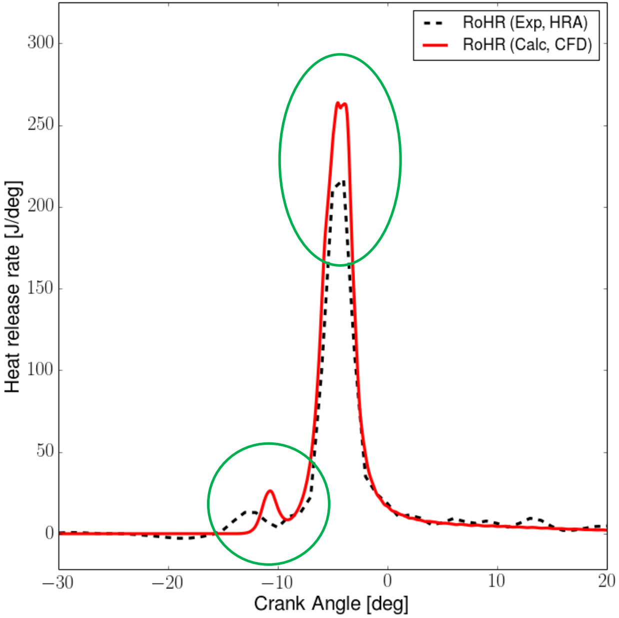
PCCI3: 3000x5



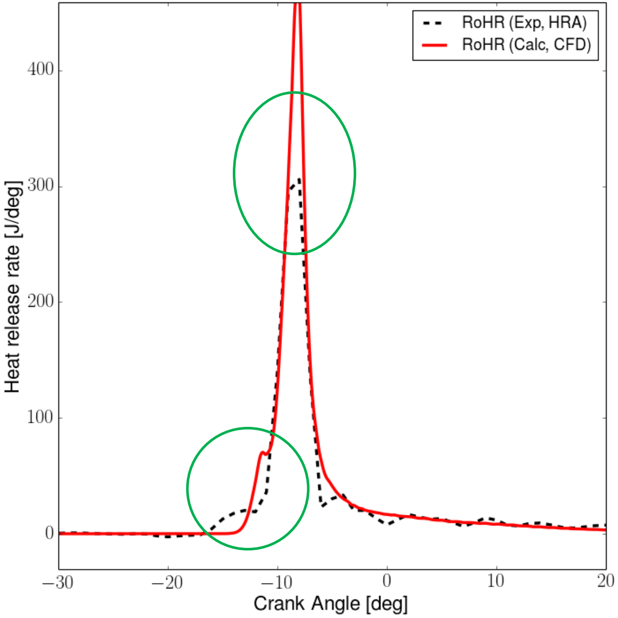
Validation: FPT F1C Engine

PCCI combustion: heat release rate

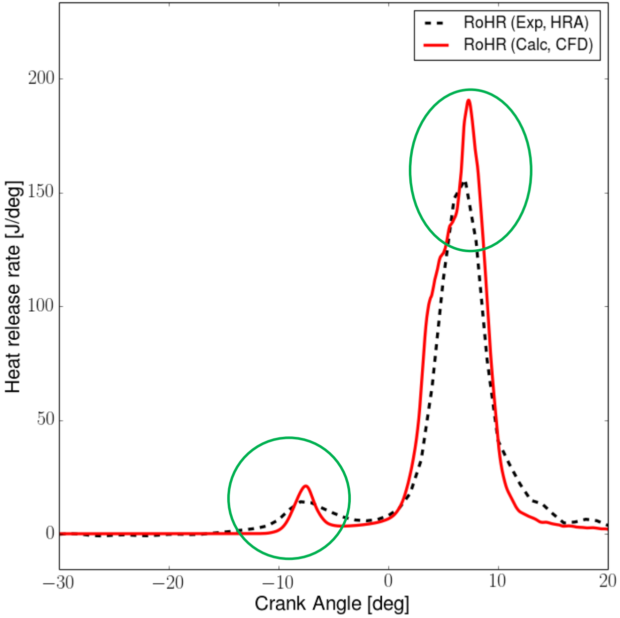
PCCI1: 2000x5



PCCI2: 2000x7.5



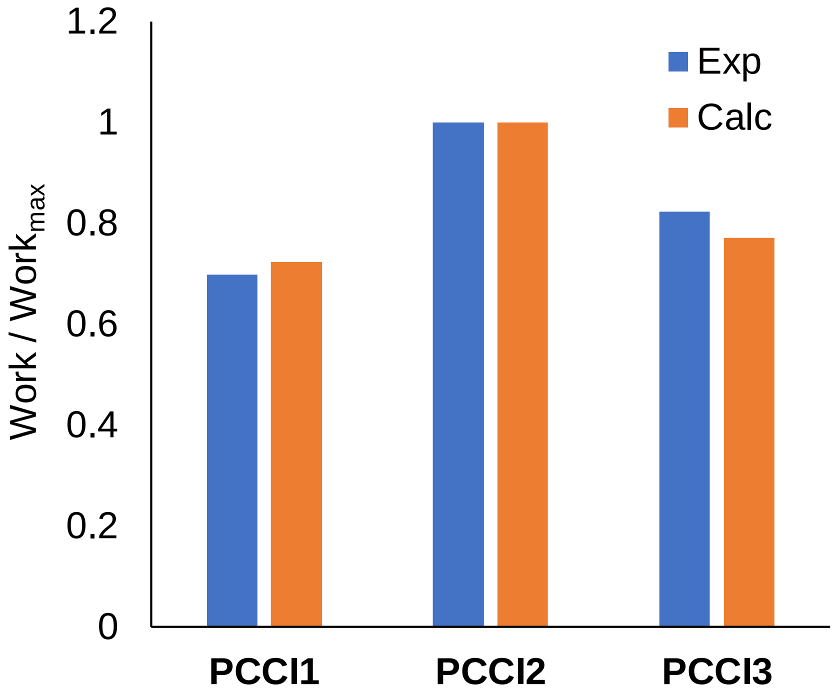
PCCI3: 3000x5



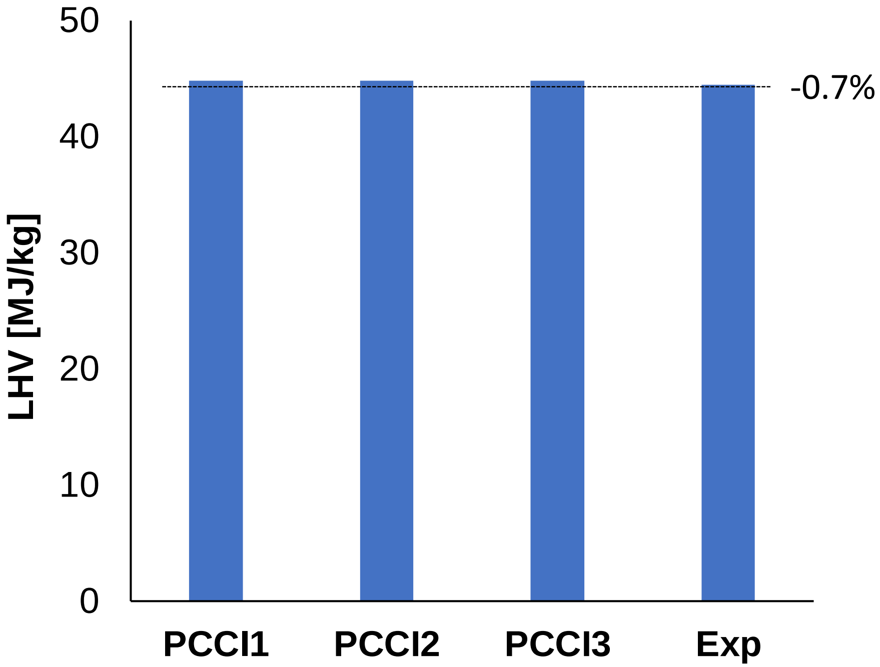
Validation: FPT F1C Engine

PCCI combustion: consistency

Gross indicated work

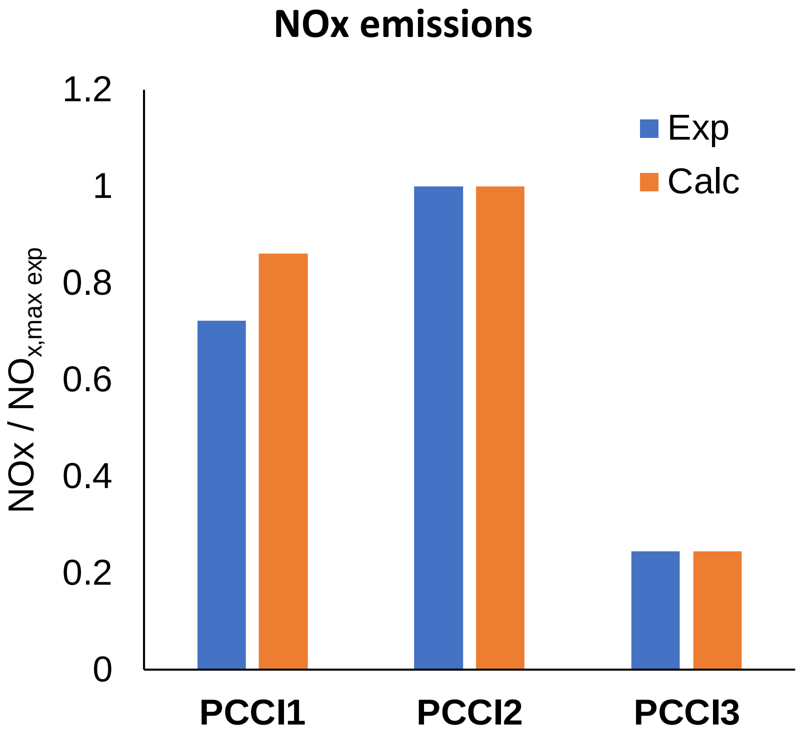


fuel LHV from cumulative heat release



Validation: FPT F1C Engine

PCCI combustion: emissions



Tabulated kinetics capable to predict PCCI combustion:

- fuel auto-ignition (cool flame + main ignition)
- peak pressure location, indicated work
- NOx emissions
- fuel energy release

To be done:

- CO emissions (kinetically controlled and not assumed to be at equilibrium conditions)

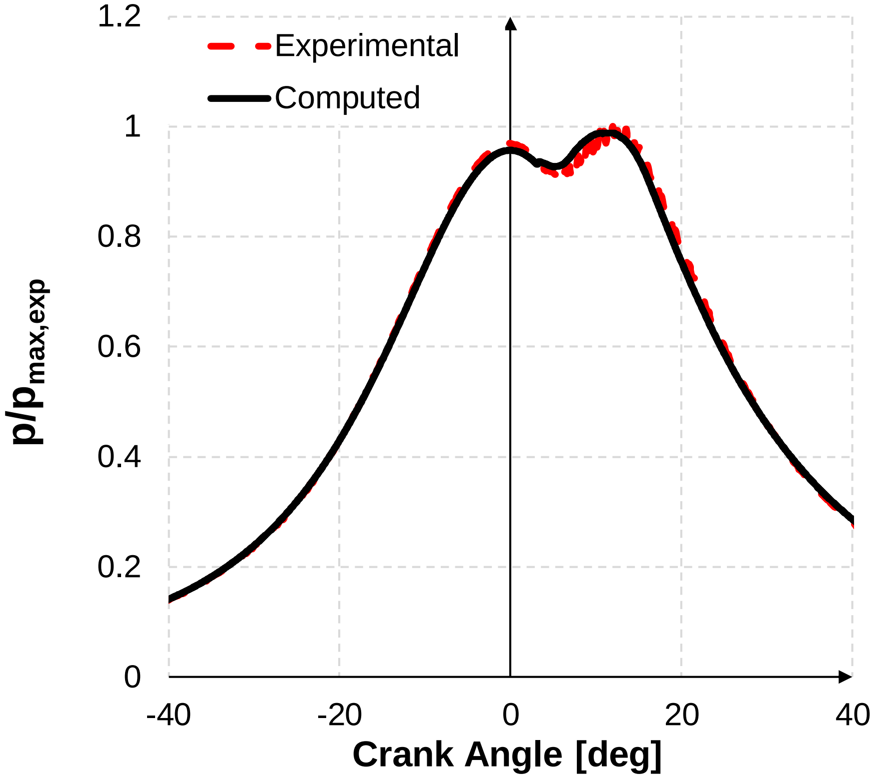
Validation: large-bore diesel engine

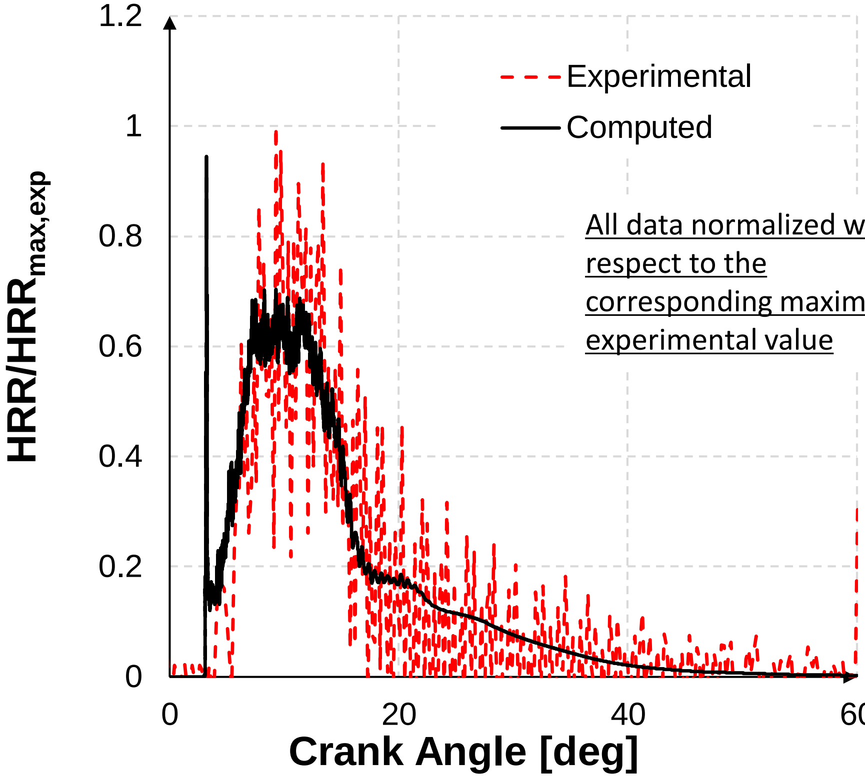
Conventional Diesel: simulation setup

	Low Load	**High Load**
SOI [CAD BTDC]	2	-2
$m_{inj}/m_{inj,full}$	0.85	1
Mesh	deforming, 650000 cells	
Fuel type	$n\text{-}C_7H_{16}$ (gas phase) IDEA (liquid properties)	
Tabulated mechanism	$n\text{-}C_7H_{16}$ from LLNL (159 species)	
Tabulation	ϕ=0.2-3; T=500-1250 K; p=2-20 MPa	

Validation: large-bore diesel engine

Conventional Diesel: validation – Low Load

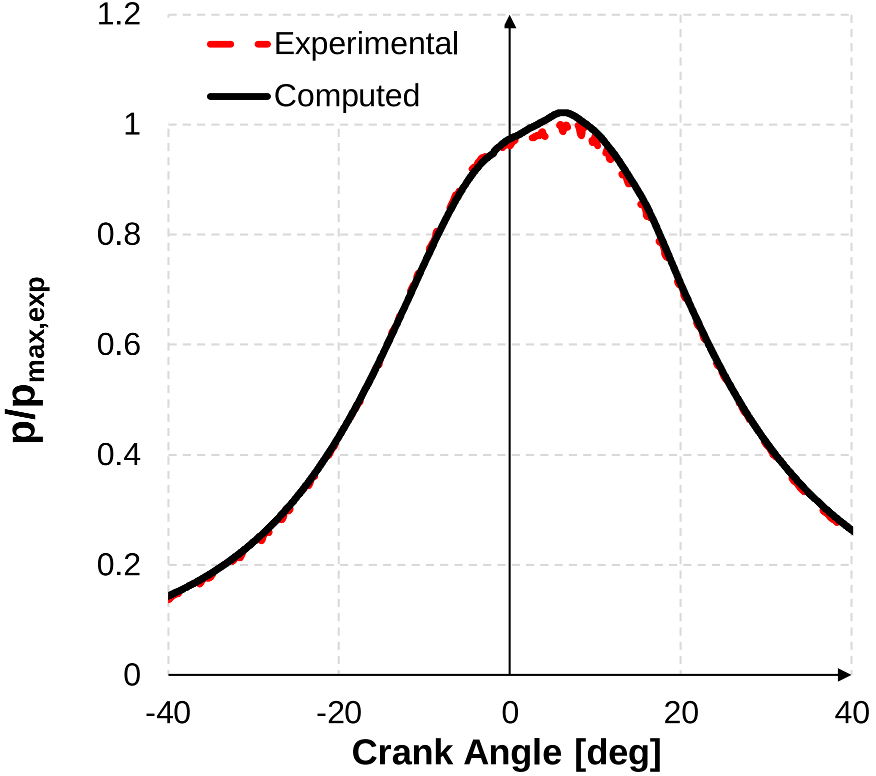


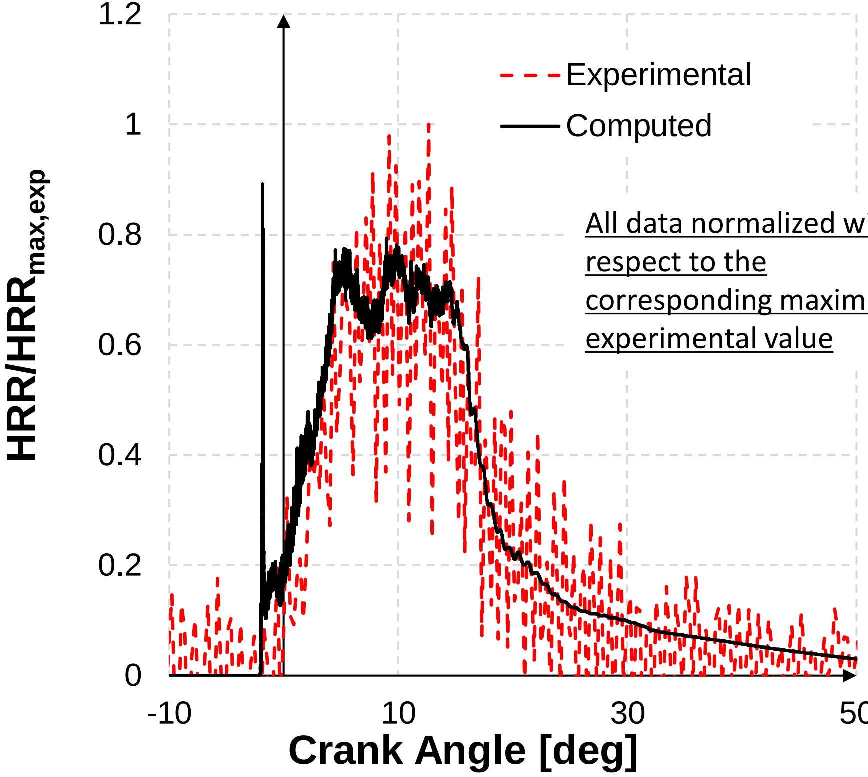


All data normalized with respect to the corresponding maximum experimental value

Validation: large-bore diesel engine

Conventional Diesel: validation – High Load





All data normalized with respect to the corresponding maximum experimental value

Validation: large-bore diesel engine

Conventional Diesel: validation

Fuel mass balance:

$$\left|\frac{\int_V \rho Z dV}{\int_{EVO} \rho dV - \int_{IVC} \rho dV}\right| < 0.2\%$$

OK!

Fuel energy balance:

$$\frac{\left(\dfrac{\int_{IVC}^{EVO} \dot{Q}_{fuel}\, d\theta}{\int_{V,EVO} \rho Z dV}\right)}{LHV_{nC_7H_{16}}} \approx 99.5\%$$

- Consistent results for single fuel mode: fundamental pre-requisite for successful dual fuel combustion simulations

Validation: large-bore diesel engine

Dual-fuel mode

Diesel fuel and natural gas directly injected into the cylinder with different SOI times

	Low Load	**High Load**
SOI Diesel [CAD BTDC]	-1	-1.5
SOI CNG [CAD BTDC]	1	0

Validation: large-bore diesel engine

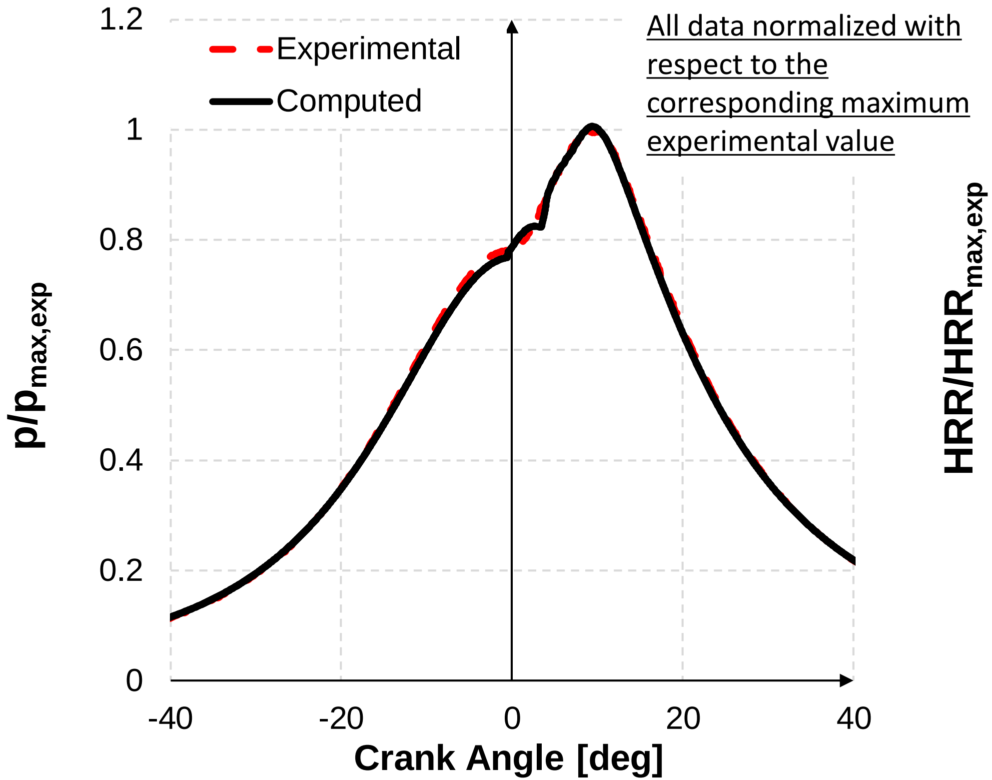
Dual-fuel mode: simulation setup

Diesel fuel type	n-C_7H_{16} (gas phase) IDEA (liquid properties)
Tabulated mechanism	n-C_7H_{16} from LLNL (159 species)
Tabulation	ϕ=0.2-3; T=500-1250 K; p = 2-20 MPa

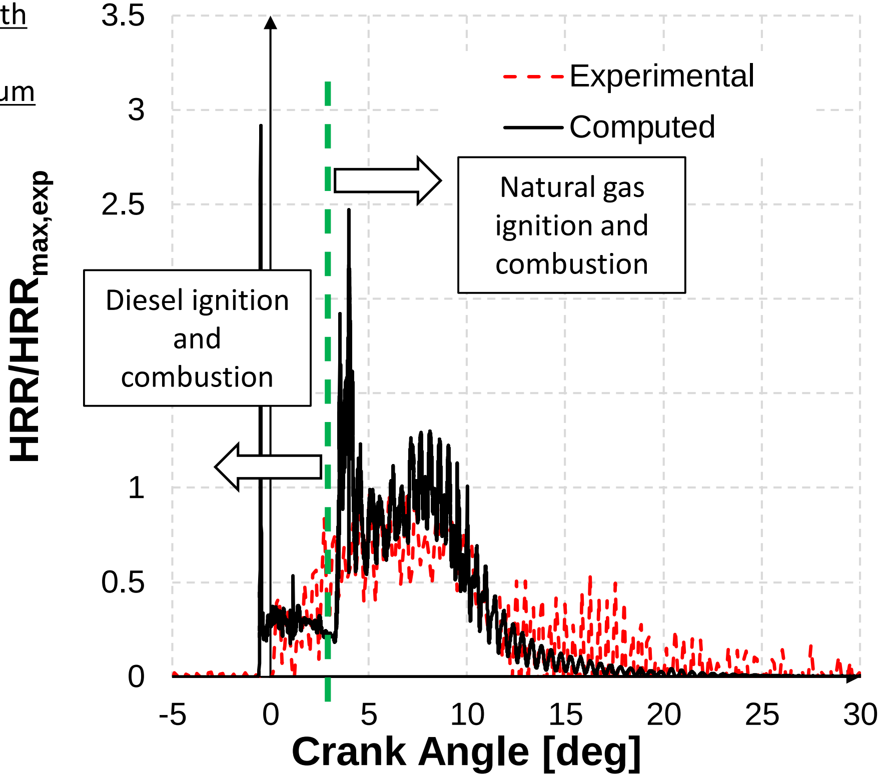
Natural gas	CH_4 (gas phase)
Tabulated mechanism	CH_4 from GRI (53 species)
Tabulation	ϕ=0.2-3; T=500-1250 K; p = 2-20 MPa

Validation: large-bore diesel engine

Dual fuel mode: Low-load condition



All data normalized with respect to the corresponding maximum experimental value

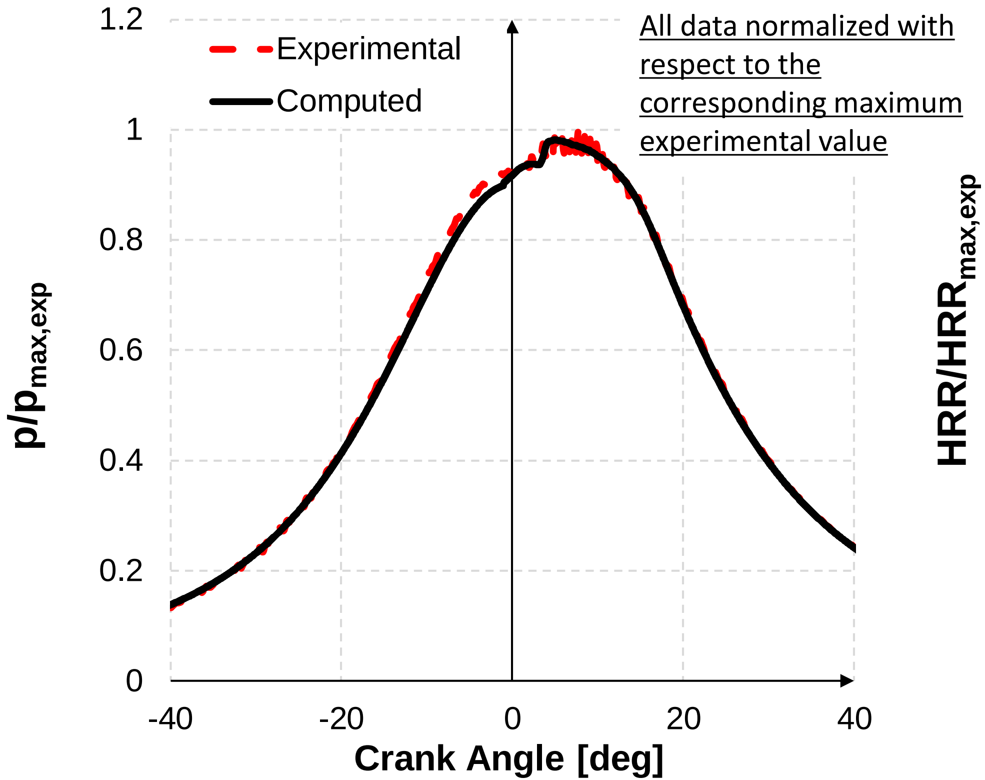


Natural gas ignition and combustion

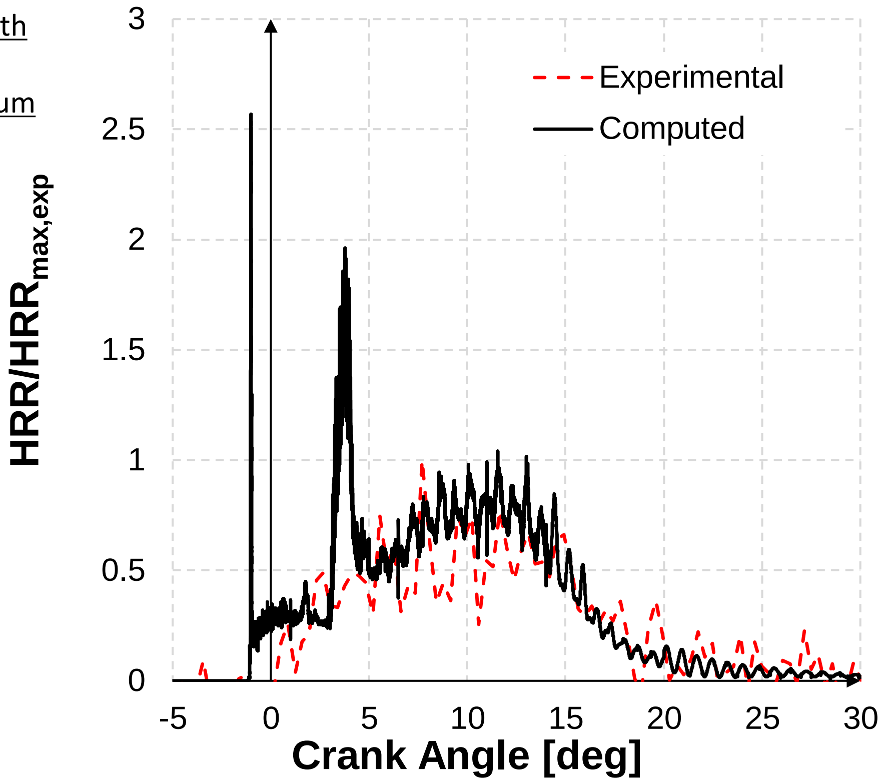
Diesel ignition and combustion

Validation: large-bore diesel engine

Dual fuel mode: High-load condition



All data normalized with respect to the corresponding maximum experimental value



Conclusions

Tabulated kinetics for combustion modeling in CI engines

Summary

- Capability to predict combustion in CI Engines:
  - Conventional Diesel
  - PCCI
  - Dual-fuel
- Consistency with respect to the energy balance

Next steps

- Dual-fuel with turbulence-chemistry interaction:
  - TPPDF
  - TFPV
- RCCI combustion
- Spark-assisted combustion

Future work

Tabulated kinetics (homogeneous reactor) combined with further complex flame structures:

- Multi-environment PDF (2 or 3 environments)
- Transported PDF

CO and HC prediction

NO_x in more complex flame structures

Heavy duty vehicles
construction, mining &
farming machinery
>90 % diesel

Passenger cars
and light duty vehicles
EU: 49% diesel

Should we rely on Diesel?

We have to, they are all around us

Ships
>95 % diesel

Locomotives
EU: 55 % diesel

**S. V. Heeb, 20th ETH conference on Combustion Genereated Nanoparticles*

Thanks for
your
attention!!!