Computational modeling of Diesel spray combustion with multiple injections

Q. Zhou, T. Lucchini, G. D'Errico

Department of Energy, Politecnico di Milano

G. Hardy

FPT Motorenforschung AG

N. Maes, B. Somers

Eindhoven University Of Technology

X. Lu

Shanghai Jiao Tong University

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Outline

1. Motivation

2. Combustion Models

- Representative Interactive Flamelet (RIF）
- Tabulated Flamelet Progress Variable (TFPV)

3. Assessment & Investigation

- Heavy-duty Diesel Engine Combustion Modeling
- Evaluation of Turbulence Models in Diesel Spray Modeling
- Diesel Spray Combustion with Multiple Injections

4. Conclusion

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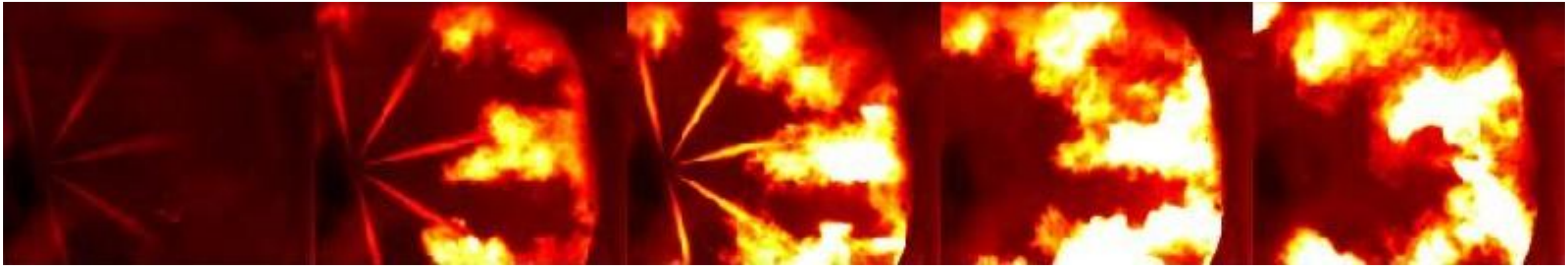
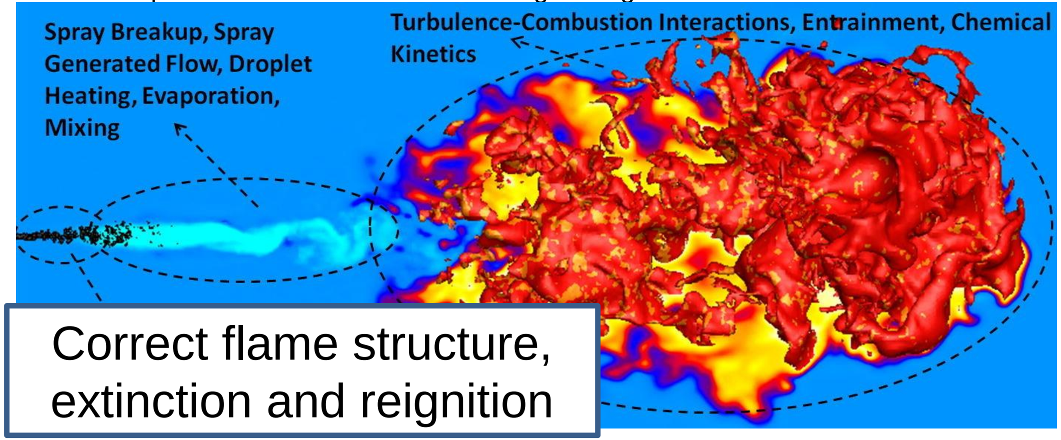
Motivation

The secret of engine...



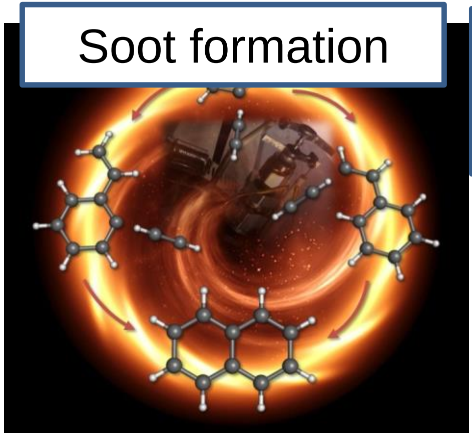
Source: https://rkdmb.home.xs4all.nl/rkd/engine/engine.html



Correct flame structure, extinction and reignition

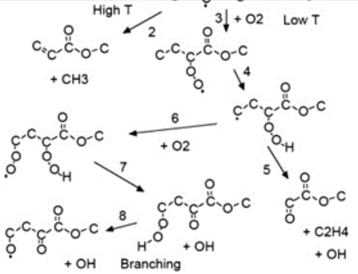
Source: Irannejad A, Banaeizadeh A, Jaberi F., Combust. Flame, 2015, 162(2): 431-450.

Soot formation



Source: Dorian Parker, University of Hawaii

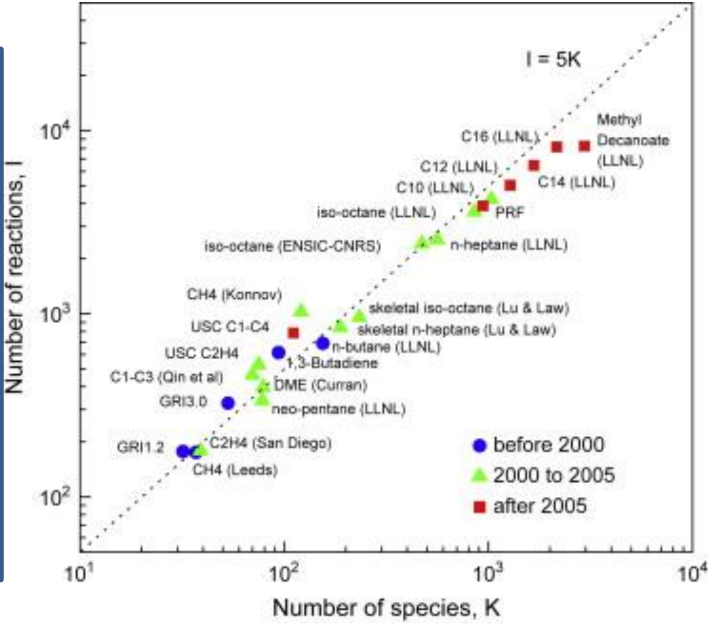
Detailed chemistry is now necessary



Motivation

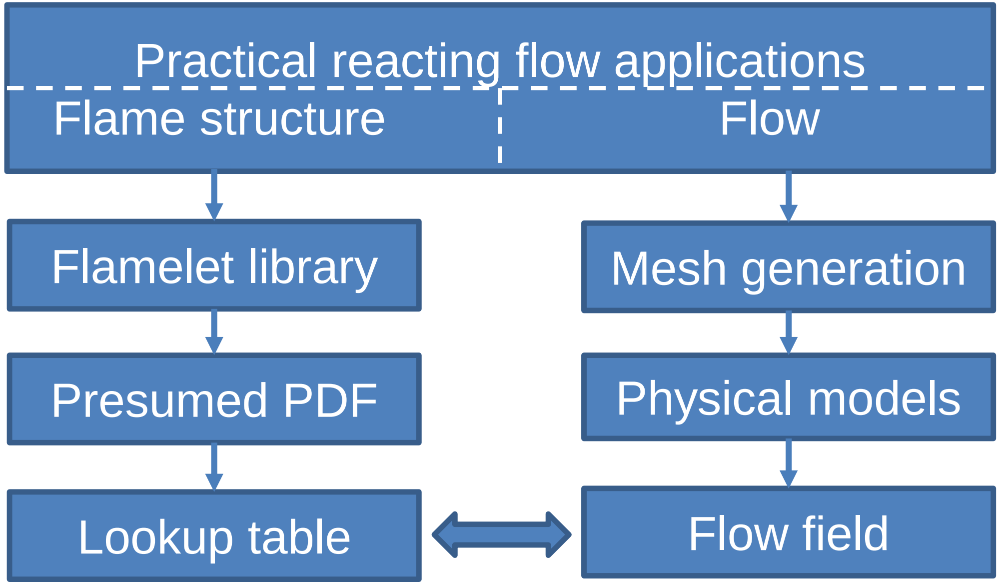
High computational burden…

Chemical source term



Transport equation & diffusion coefficients

Solution: Tabulated Kinetics



Practical reacting flow applications

Flame structure

Flow

Flamelet library

Presumed PDF

Lookup table

Mesh generation

Physical models

Flow field

For Diesel combustion, the TFPV, assuming unsteady diffusion flame, will be presented

Source: Lu and Law, Prog. Energ. Combust. (2009), C K. Law, P COMBUST INST. (2007).

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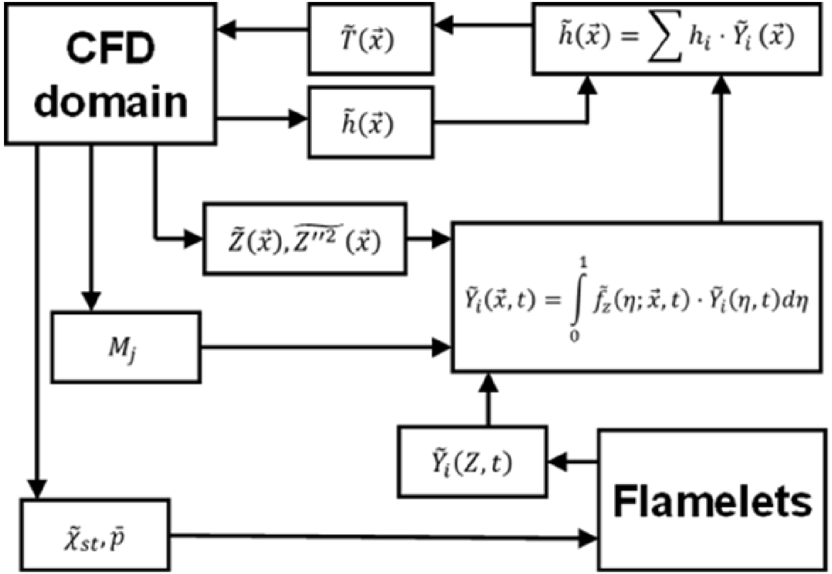
RIF

Laminar flamelet concept describes diffusion flame



CFD domain

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

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

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

$\tilde{Z}(\vec{x}), \widetilde{Z''^2}(\vec{x})$

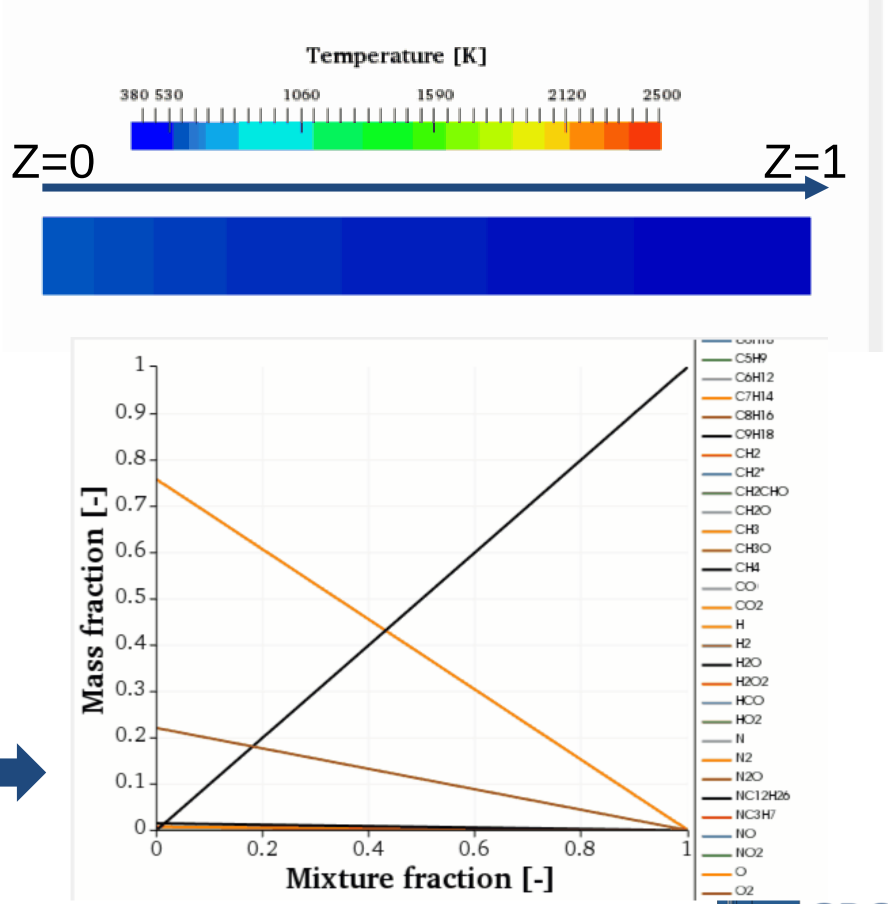
$\tilde{Y}_i(\vec{x},t) = \int_0^1 \tilde{f}_Z(\eta;\vec{x},t) \cdot \tilde{Y}_i(\eta,t)\,d\eta$

M_j

$\tilde{Y}_i(Z,t)$

$\tilde{\chi}_{st}, \bar{p}$

Flamelets

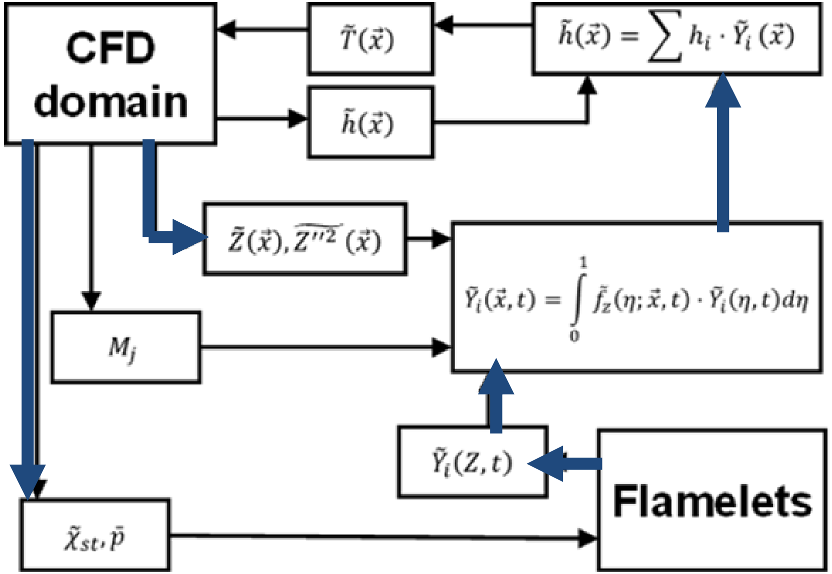


RIF

1: transport equation in CFD domain

2: flamelet equation and pdf integration

3: update composition in CFD domain



CFD domain

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

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

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

$\tilde{Z}(\vec{x}), \widetilde{Z''^2}(\vec{x})$

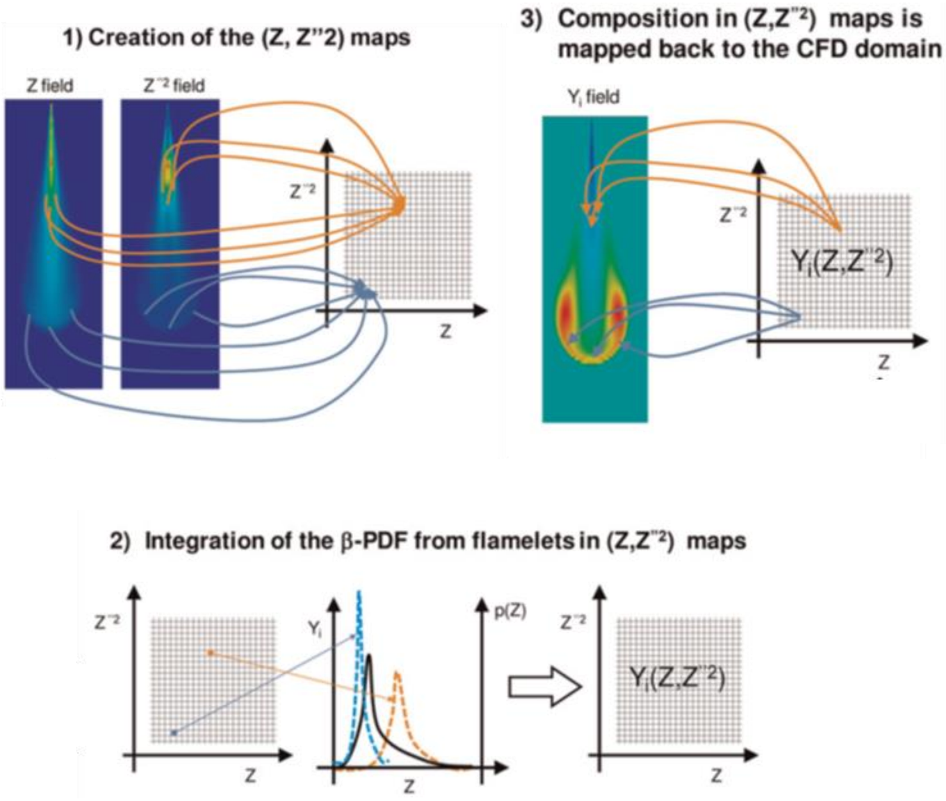
$$\tilde{Y}_i(\vec{x},t) = \int_0^1 \tilde{f}_Z(\eta;\vec{x},t) \cdot \tilde{Y}_i(\eta,t)\,d\eta$$

M_j

$\tilde{Y}_i(Z,t)$

Flamelets

$\tilde{\chi}_{st}, \tilde{p}$



1) Creation of the (Z, Z''2) maps

3) Composition in (Z,Z''2) maps is mapped back to the CFD domain

2) Integration of the β-PDF from flamelets in (Z,Z''2) maps

Source: D'Errico, G., Lucchini, T., Onorati, A., & Hardy, G. (2014). International Journal of Engine Research, 16(1), 112–124.

HR Table

Homogenous chemistry table:

Mechanism, Initial conditions (p, T_w, EGR, ϕ)

↓

0D homogenous reactor solver

↓

Homogenous lookup table (progress variable reaction rate & compositions)

Progress Variable definition:

reconstruction of the thermo-chemical state on the whole reaction trajectory

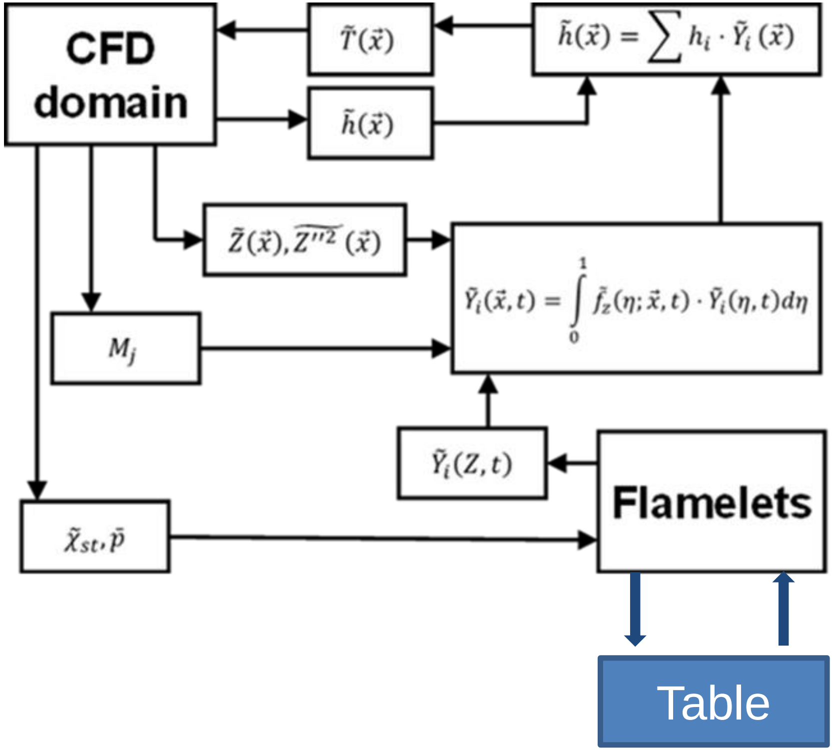
$$C = \sum_{i=1}^{Ns} h_{298,i} \cdot (Y_i(t) - Y_i(0))$$

- C is equal to the heat released by combustion
  - C=0: unburned mixture
  - C=1: fully burned mixture
- Track both low and high temperature reactions
- uniquely characterizes each point in the thermochemical state space and is appropriate for a transport equation.

Definition adopted from: Lehtiniemi et al., Combust Sci Technol 178, 2006

TRIF

Tabulated **RIF**



Flamelet domain

Flamelet equation:

$$\cancel{\rho \frac{\partial h}{\partial t} = \rho \frac{\chi_Z}{2} \frac{\partial^2 h}{\partial Z^2} + \frac{dp}{dt}} \qquad \cancel{\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi_Z}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i}$$

$$\rho \frac{\partial h_u}{\partial t} = \rho \frac{\chi_Z}{2} \frac{\partial^2 h_u}{\partial Z^2} + \frac{dp}{dt} \qquad \rho \frac{\partial C}{\partial t} = \rho \frac{\chi_Z}{2} \frac{\partial^2 C}{\partial Z^2} + \dot{C}$$

Z, T, p, C

$Y_i \& \dot{c}$

Chemistry table (0 D homogeneous reactor calculations)

TFPV

CFD solver

Mixture fraction

$$\frac{\partial \bar{\rho} \tilde{Z}}{\partial t} + \nabla(\bar{\rho} \tilde{U} \tilde{Z}) - \nabla(\tilde{\mu}_t \nabla \tilde{Z}) = \dot{S}_Z$$

Mixture fraction variance

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

Stoichiometric scalar dissipation rate

$$\chi_{st} = \frac{\chi}{\int_0^1 \frac{f(Z)}{f(Z_{st})} \tilde{P}(Z) dZ}$$

Progress variable

$$\frac{\partial \bar{\rho} \tilde{C}}{\partial t} + \nabla(\bar{\rho} \tilde{U} \tilde{C}) - \nabla\left(\frac{\tilde{\mu}_t}{Sc_t} \nabla \tilde{C}\right) = \bar{\rho}\dot{C}$$

Unburned gas enthalpy

$$\frac{\partial \bar{\rho} \widetilde{h_u}}{\partial t} + \nabla(\bar{\rho} \tilde{U} \widetilde{h_u}) - \nabla(\widetilde{\alpha_t} \nabla \widetilde{h_u}) = \dot{Q}_s + \frac{\bar{\rho}}{\bar{\rho}_u} \cdot \frac{D\bar{p}}{Dt}$$

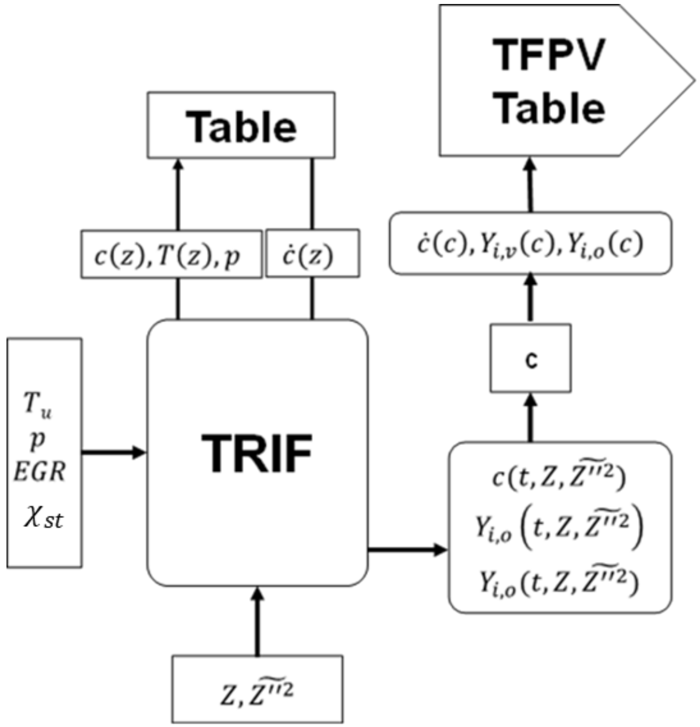
$\tilde{Z}, \widetilde{Z''^2}, \chi_{st}$

c, p, Tu

$Y_i \& \dot{c}$

Lookup table

(unsteady diffusion flame calculations)



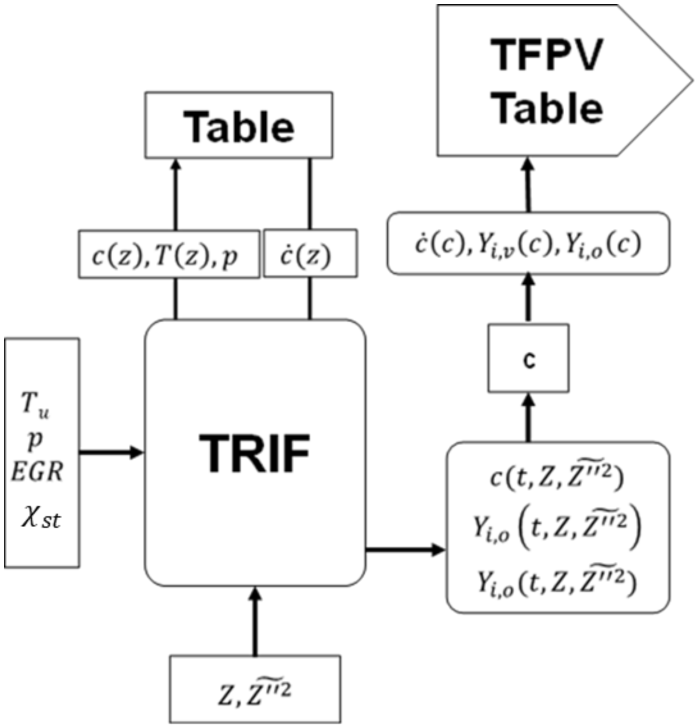
Expectations

Compared to RIF using a single flamelet formulation, TFPV model is to provide a realistic description of the turbulent diffusion flame, especially in the presence of multiple injections:

- Extinction in the near-nozzle region where the scalar dissipation rate is very high;
- Re-ignition due to progress variable convection and diffusion;
- Flame stabilization process including effects of both premixed and diffusive flame propagation.

Lookup table

(unsteady diffusion flame calculations)



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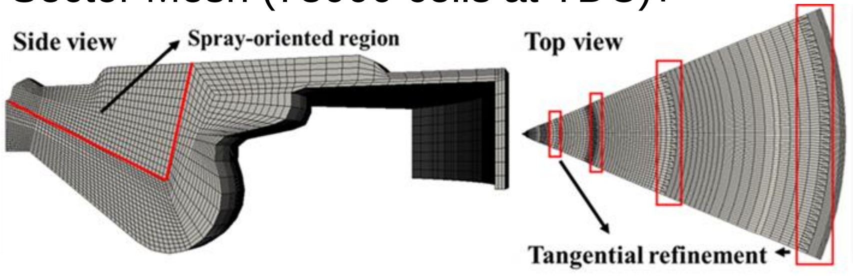
Heavy-Duty Engine: case setup

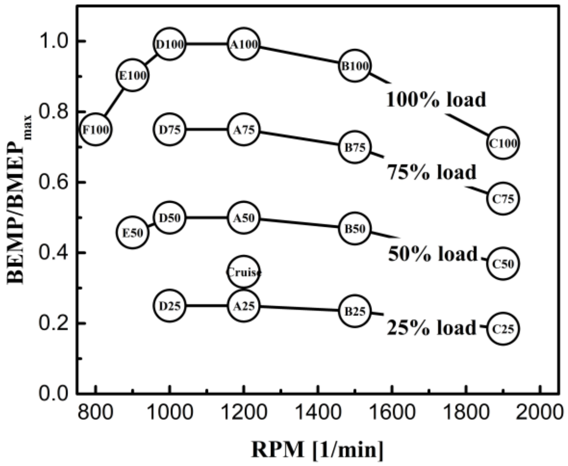
Sector Mesh (73000 cells at TDC):



Engine Specifications:

Bore	128 mm
Stroke	144 mm
Compression ratio	20.5:1
Injector holes	8
Injection cone angle	146°
#injection	1

Simulated operating conditions:



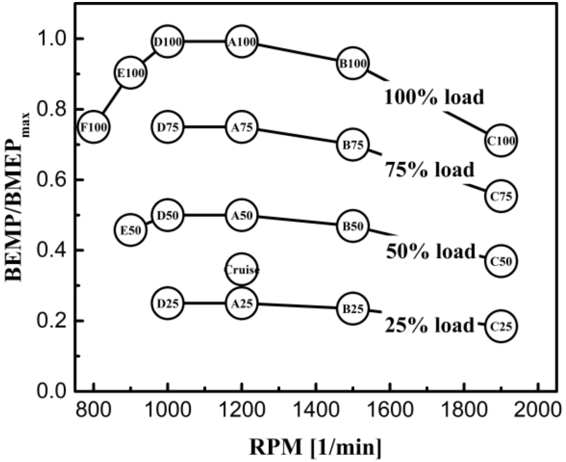
Chemistry table discretization:

Temperature [K]	400, 450, 500, 550, 600, 650, 700, 750, 800, 850, 900, 950, 1000, 1050, 1100, 1150, 1250
Pressure [bar]	20, 60, 100, 150, 200, 250
Equivalence ratio [-]	0, 0.2, 0.4, 0.5, 0.6, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95, 1, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3, 1.35, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2, 2.2, 2.4, 2.6, 2.8, 3, 3.5, 1e15
Mixture fraction variance segregation [-]	0, 0.001, 0.005, 0.01, 0.05, 0.1, 1.0
Scalar dissipation rate [1/s]	0, 1, 3, 7, 20, 55, 100

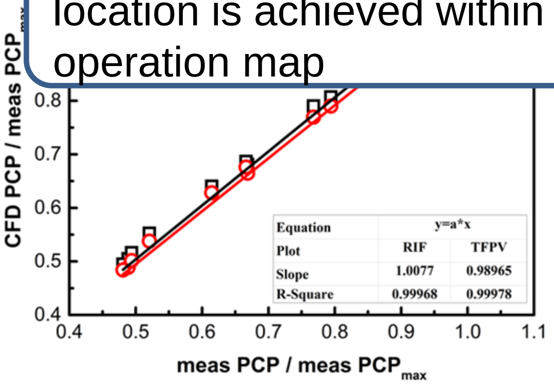
Three chemistry tables were generated, each one for operating points with similar oxidizer chemical compositions at IVC.

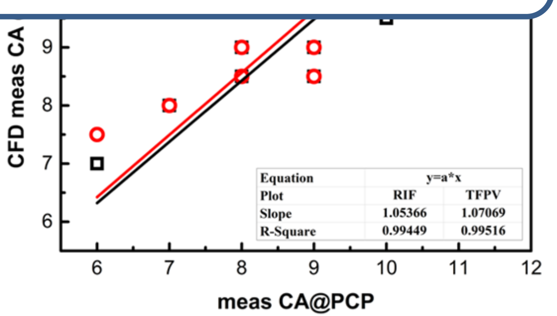
Heavy-Duty Engine: summary

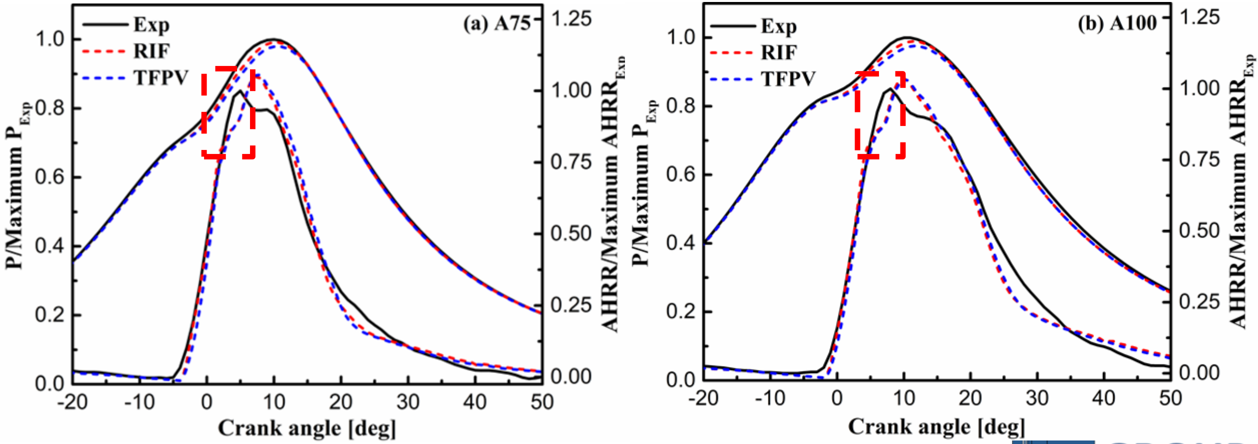
Simulated operating conditions:



Very good prediction of Peak Cylinder Pressure and its location is achieved within a wide range of engine operation map







1. Improve flame wall interaction using $k-\omega\ SST$ model
2. Compare RIF and TFPV in presence of multiple injection

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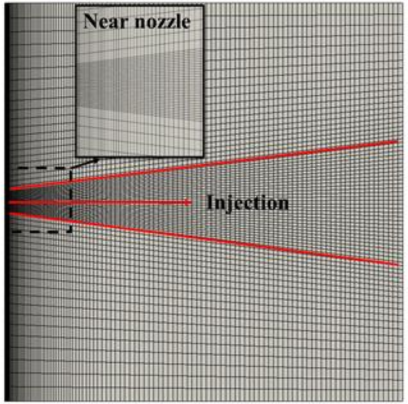
Spray A case setup



108 mm cube
$\boldsymbol{k-\omega}$ **SST:** 1.0 M cells, much refined near nozzle
$\boldsymbol{k-\varepsilon}$**:** 0.4 M cells

$\boldsymbol{k-\omega}$ SST case

- hollow cone injector
- Reitz-Diwakar breakup
- standard $k-\omega$ SST with modified γ_2
- Frassodati, 130 species & 2323 reactions

$\boldsymbol{k-\varepsilon}$ case

- hollow cone injector
- Reitz-Diwakar breakup
- standard k-ε with modified C_1
- Frassodati, 130 species & 2323 reactions

Chemistry table discretization

Temperature [K]	400, 450, 500, 550 600, 650, 700, 750, 800, 850, 900, 1000, 1050, 1150, 1250, 1350
Pressure [bar]	45, 55, 65
Equivalence ratio	0, 0.2, 0.4, 0.5, 0.6, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95, 1, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3, 1.35, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2, 2.2, 2.4, 2.6, 2.8, 3, 3.5, 1e15
Mixture fraction segregation	0, 0.001, 0.005, 0.01, 0.05, 0.1, 1
Scalar dissipation rate [1/s]	0, 1, 3, 7, 20, 55, 100

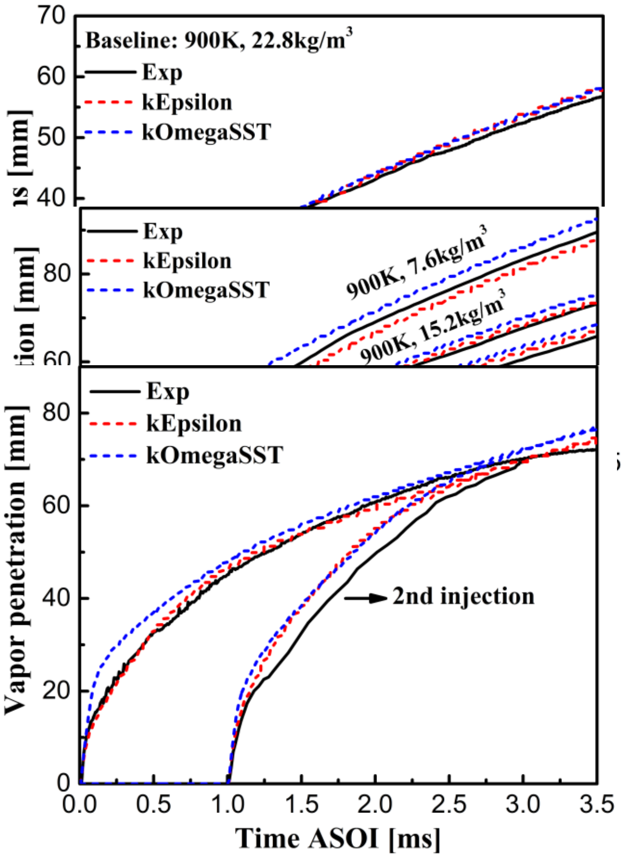
Non-reacting: liquid and vapor penetration

Simulated operating conditions

Op	T_{amb} [K]	ρ_{amb} [kg/m^3]	P_{inj} [bar]	Injection Strategy [ms]	[O2]	Injector
1	900	22.8	1500	1.5	0%	#210370
2	900	15.2	1500	1.5	0%	#210370
3	900	7.6	1500	1.5	0%	#210370
4	700	22.8	1500	1.5	0%	#210370
5	900	22.8	1500	0.5/ 0.5 dwell/ 0.5	0%	#210370
6	900	22.8	1500	0.5/ 0.5 dwell/ 0.5	15%	ECN#306.22
7	900	22.8	1500	0.5/ 0.5 dwell/ 0.5	15%	#210370

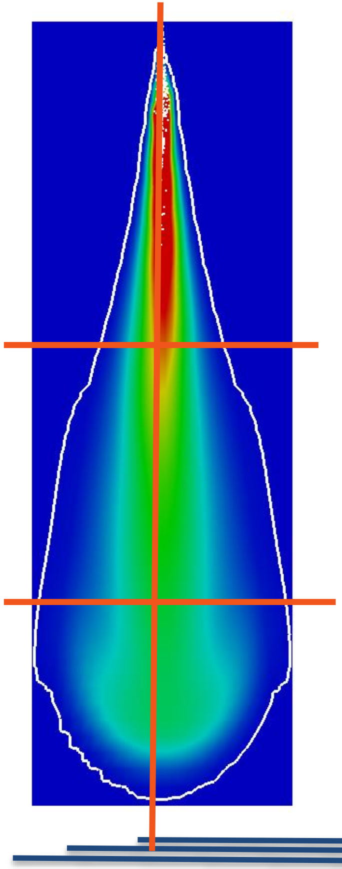
$k-\omega\ SST$ slightly overpredict the vapor penetration at the initial stage (0.15 ms) where liquids exit.

The accuracy is adequate since turbulent spray flames take place after the transient liquid penetration

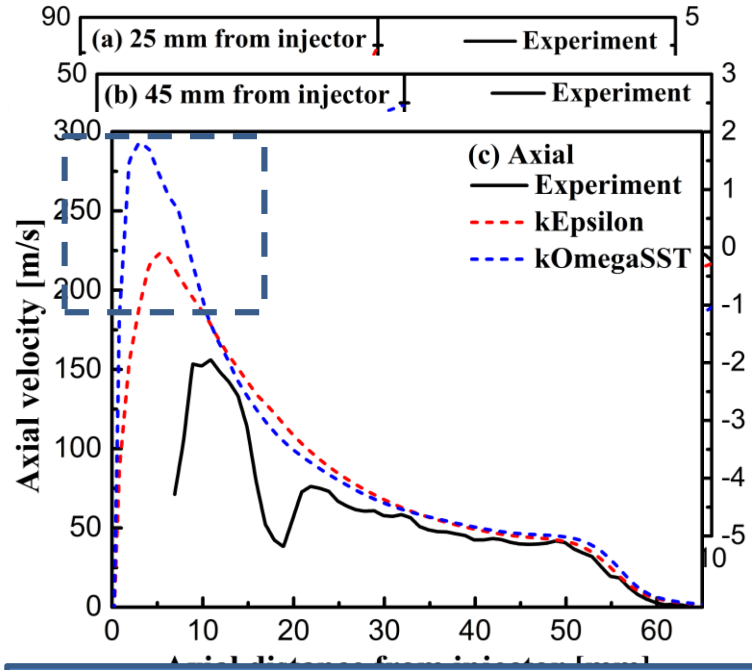


Non-reacting: velocity and mixture fraction

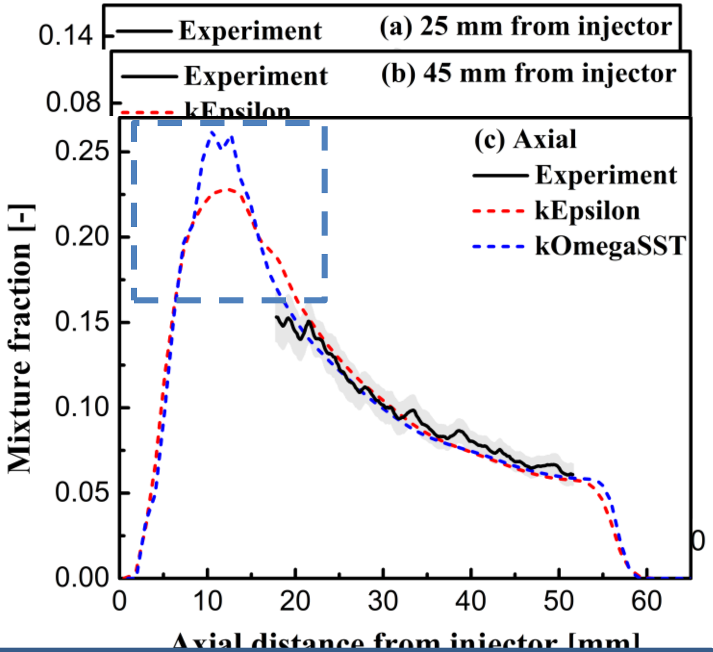
Op1@1.5 ms ASOI



Velocity



Mixture fraction



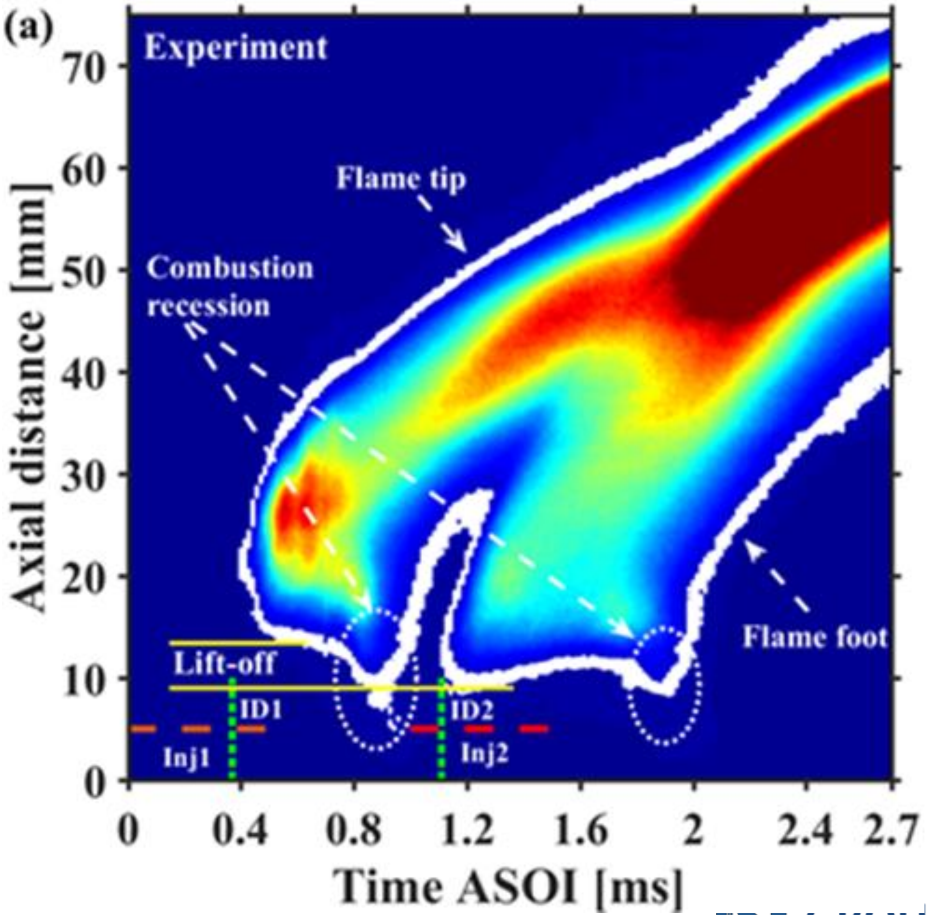
Differences between the distributions predicted by $k-\varepsilon$ and $k-\omega\ SST$ models occur along the centerline of the spray, approximately from 10 mm to 15 mm

Reacting: $I{-}x{-}t$ plot

$I - x - t$ (intensity - axial distance - time) is calculated by integrating OH* chemiluminescence data from experiments or OH mass fraction from CFD along the symmetry axis

Features are shown in such plot:

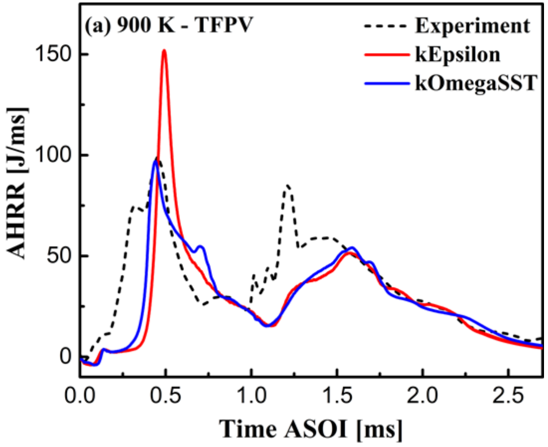
1. Ignition delay
2. Lift-off length
3. High temperature combustion recession
4. Flame tip and foot

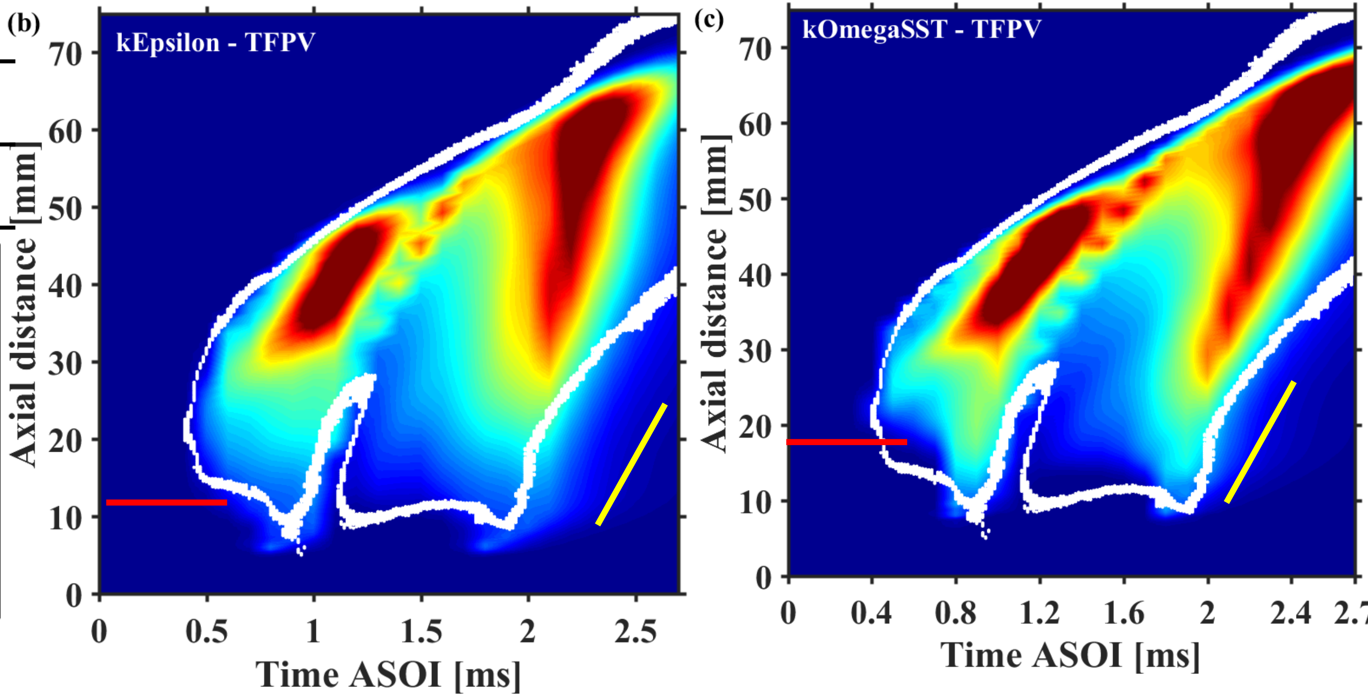


Reacting (TFPV): $k-\varepsilon$ vs. $k-\omega\ SST$

Ignition delay

Exp. [ms]	$k-\omega$ SST	$k-\varepsilon$
0.37±0.1 /0.11±0.08	0.44/0.15	0.47/0.16





1. $k-\omega\ SST$ predicts longer lift-off due to richer mixture and higher velocity near injector

2. Similar description in terms of flame tip, while $k-\omega\ SST$ better captures the burn-out

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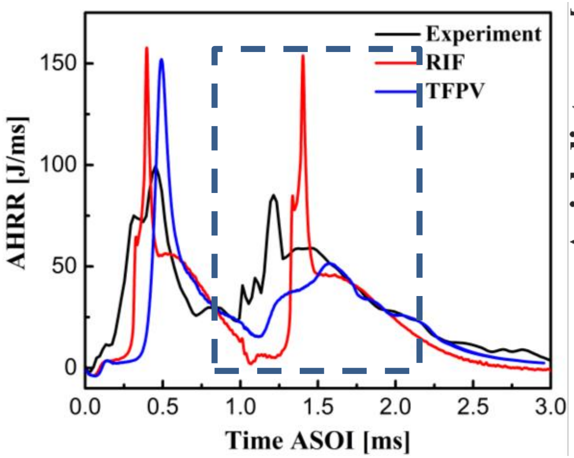
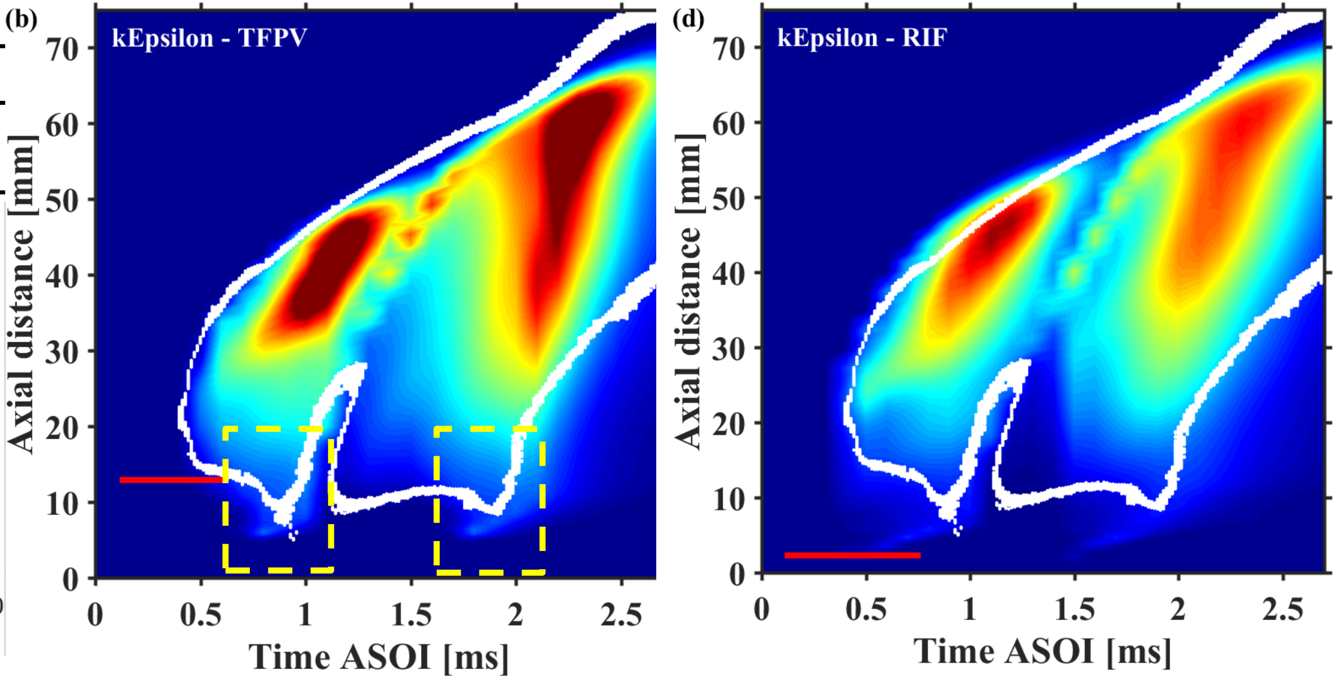
Spray A: high-temperature reactions

Ignition delay

Exp. [ms]	RIF	TFPV
0.37±0.1 /0.11±0.08	0.39/0.24	0.47/0.16



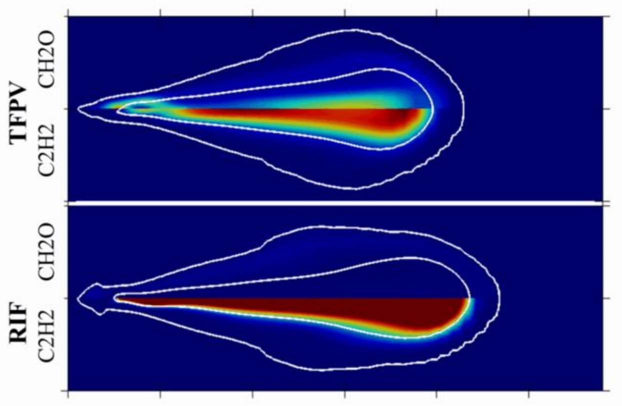


1. The progress variable approach gives better description of ignition and combustion of the second injection event;

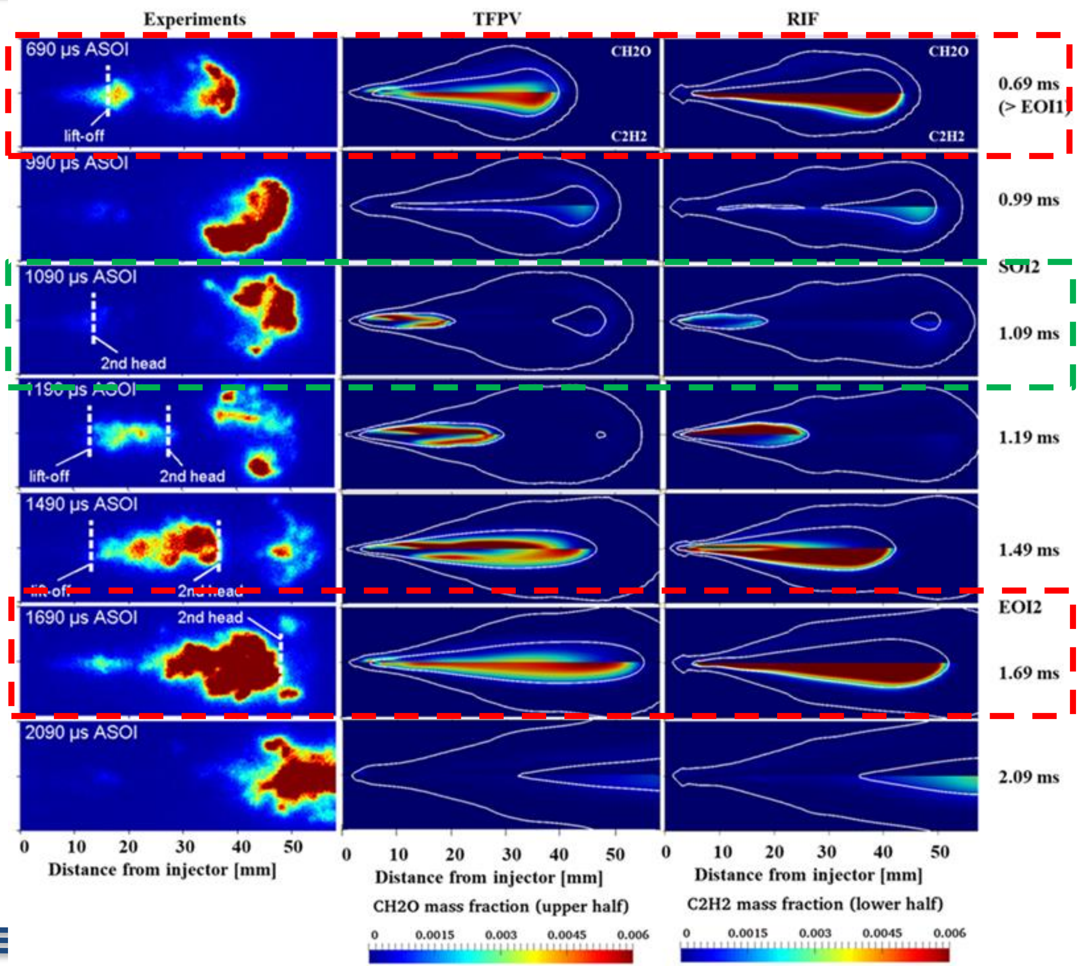
2. TFPV could correctly predict the lift-off and combustion recession

Spray A: low-temperature reactions

Capability of capturing the cool flame characteristics and tracking low-temperature products formaldehyde (CH_2O)

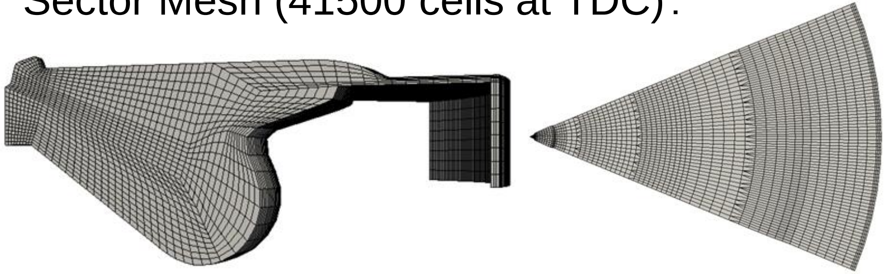


1. 0.69 and 1.69 ms: The low-temperature combustion recession was observed in TFPV case
2. 1.09 ms: TFPV predicts more distinct CH2O in the near nozzle region



Light-Duty Engine: case setup

Sector Mesh (41500 cells at TDC):

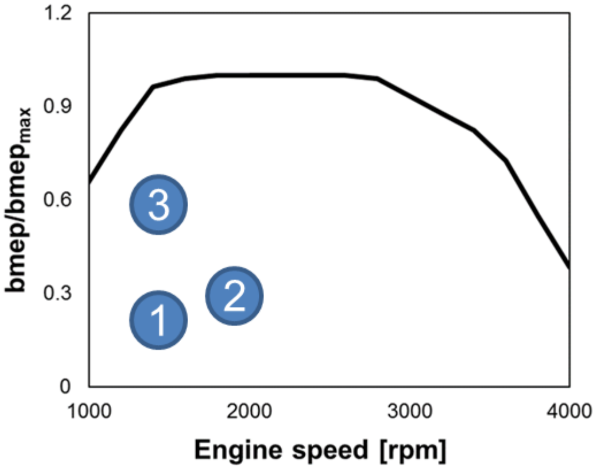


Engine Specifications:

Bore	96 mm
Stroke	105 mm
Compression ratio	18:1
Injector holes	8
Injection cone angle	130°

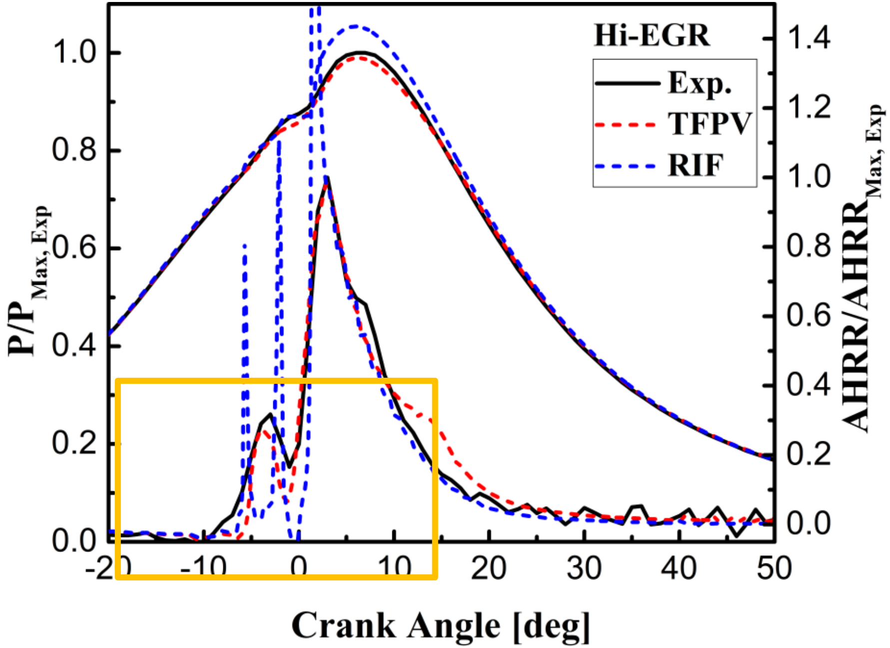
Simulated operating conditions:

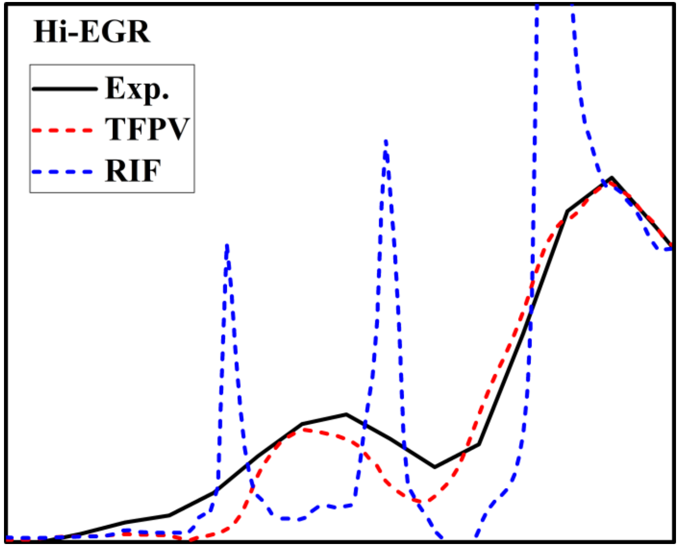
	Hi-EGR	A25	1400X9
Speed [rpm]	1400	2000	1400
Load [%]	25	25	50
#injections	3	3	3
EGR [%]	40	22	14
λ	2.3	1.85	1.2



3 low load operation conditions, where pilot injections are present, were chosen.

Light-Duty Engine: Hi-EGR

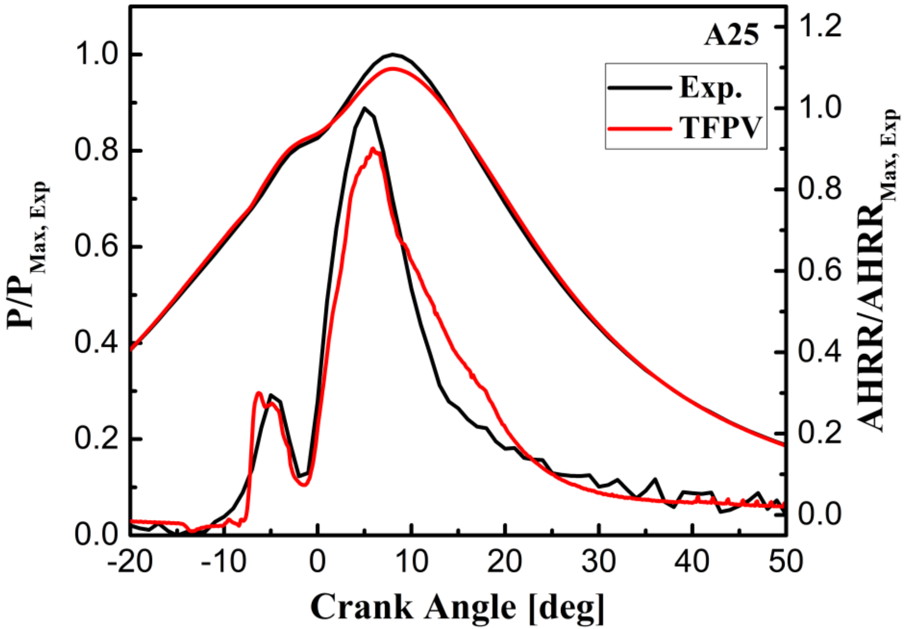


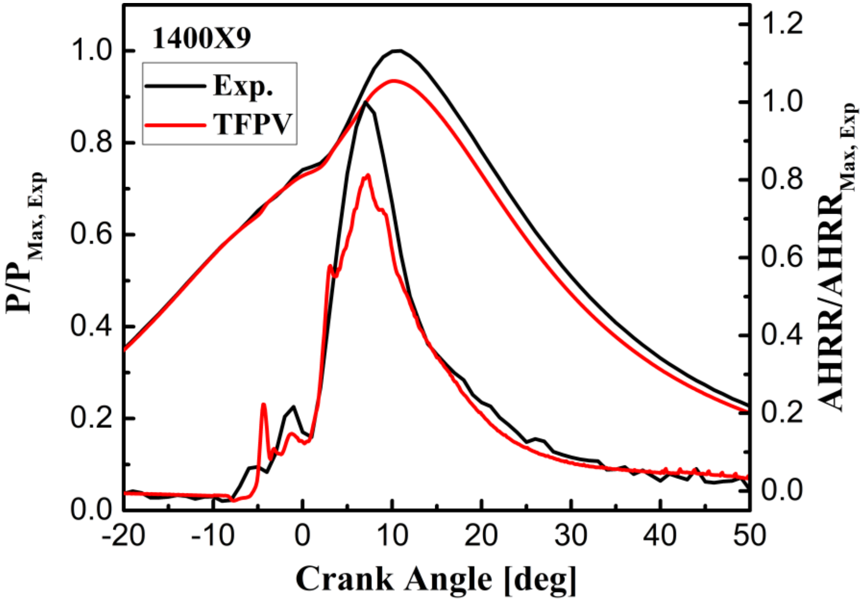


TFPV achieves better agreement with experiments in terms of pressure & AHRR

Similar to Spray A case, the progress variable approach predicts smoother AHRR

Light-Duty Engine: A25 & 1400X9





For A25 case, TFPV could predict the pressure and AHRR very well, while further investigation should be conducted for 1400X9 case.

Outline

1. **Motivation**
2. **Combustion Models**
   - Representative Interactive Flamelet (RIF）
   - Tabulated Flamelet Progress Variable (TFPV)
3. **Assessment & Investigation**
   - Heavy-duty Diesel Engine Combustion Modeling
   - Evaluation of Turbulence Models in Diesel Spray Modeling
   - Diesel Spray Combustion with Multiple Injections
4. **Conclusion**

Conclusion

TFPV vs. RIF:

1. Both models could provide encouraging results in heavy-duty engine application, when only one main injection is used.
2. The advantages of TFPV become more evident in the presence of multiple injections:
   - ➢ Ignition delay and AHRR of the second injection event (Spray A)
   - ➢ Lift-off, low- and high-temperature combustion recession (Spray A)
   - ➢ Pressure and AHRR (LD engine)

$\boldsymbol{k-\omega\ SST}$ vs. $\boldsymbol{k-\varepsilon}$ model:

1. The $k-\omega\ SST$ could give a comparable prediction with respect to $\mathrm{k}-\varepsilon$ in both non-reacting (liquid and spray penetration, mixture fraction and velocity distribution) and reacting case.

Next step:

1. Comprehensive validation of TFPV in LD engine with multiple injections
2. Use of $k-\omega\ SST$ in practical engine applications

Thanks for your attention!!!