Fourth Two-Day Meeting on IC engine Simulations using the OpenFOAM technology

Modeling of premixed combustion in conventional and innovative engines

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Methodology

Combustion model:
- Initial flame development → Herweg and Maly 0-D model
- Turbulent flame propagation → Weller model
- Burned gas chemical composition → Tabulated kinetics
- Laminar flame speed → Correlations or tabulation

Validation

Constant-volume vessel
- Initial flame development and transition to flame propagation

GDI optical engine
- Charge motions effects

Natural gas engines
- Influence of mesh (2d vs 3d) and combustion model

Advanced concepts

Dual fuel combustion:
- Auto-ignition+premixed flame propagation: proposed models
- Preliminary validation: heavy-duty engine

Prechamber combustion (turbulent jet ignition):
- Flame propagation under different regimes
- Preliminary validation at constant-volume conditions

Lib-ICE

Modeling IC Engines using the OpenFOAM technology

In-cylinder

- Gas exchange
- Fuel air mixing (Direct-injection, PFI, liquid, gas)
- Combustion (spark-ignition, compression-ignition, HCCI, PCCI, RCCI, ...)

Intake/exhaust

- 1D-3D coupling (Gasdyn+OpenFOAM coupling)
- Exhaust aftertreatment system: SCR, Three-way catalyst, DPF, GPF, ...

Applications

- design/development
- investigation of complex process in IC engines: reactive, turbulent, compressible and multiphase flows

Why OpenFOAM?

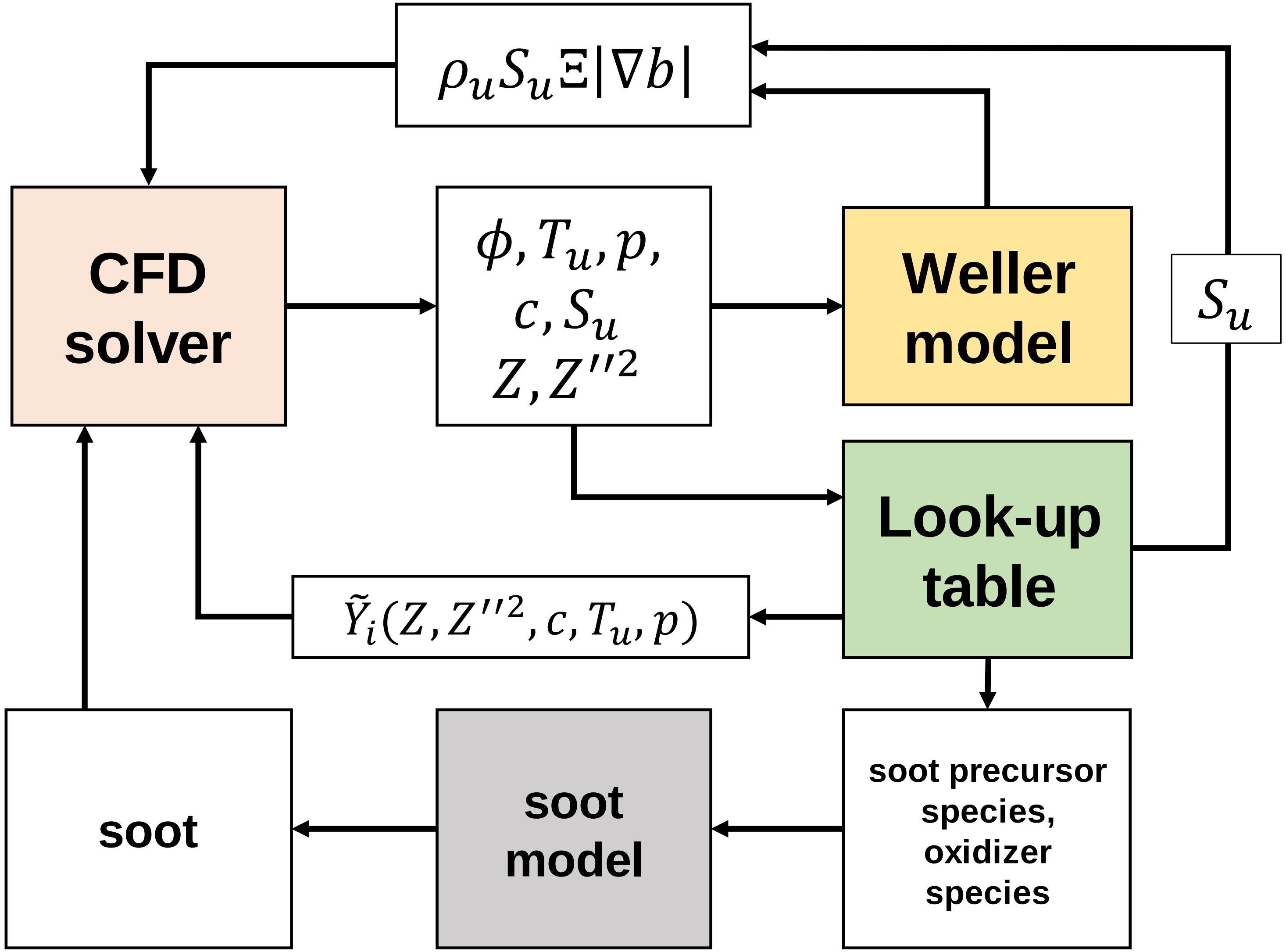
Potential for development

Advanced models required by the engines of the future

Simulation methods

Combustion model: methodology

- CFD domain: main transport equations + mixture fraction and regress variable
- Weller model: regress variable source term
- Tabulated kinetics:
  - Burned gas chemical composition (including soot precursors)
  - Laminar flame speed
- Soot model: semi-empirical



Combustion model

Regress variable transport equation

$$\frac{\partial \rho b}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} b) - \nabla \cdot (\mu_t \nabla b) = \rho_u S_u \Xi |\nabla b| + \dot{\omega}_{ign}$$

- b : unburned gas mass fraction
- Ξ : flame wrinkle factor (S_t/S_u)
- S_u : laminar flame speed
- $\dot{\omega}_{ign}$: ignition source term

Ignition: deposition model

$$\dot{\omega}_{ign} = \frac{C_s \rho_u b}{\Delta t_{ign}}$$

- C_s : user-defined
- Δt_{ign} ignition duration
- ρ_u : unburned gas density

Turbulent combustion: Weller model

1) **Algebraic expression**: $\Xi = 1 + f \cdot \left(\Xi_{eq} - 1\right)$

- Global transition factor f to describe laminar to turbulent flame propagation
- Equilibrium wrinkle factor from Gulder correlation:

$$\Xi = \Xi_{eq}^{*} = 1 + C_{\Xi} \cdot \sqrt{u'/S_u} R_{\eta}$$

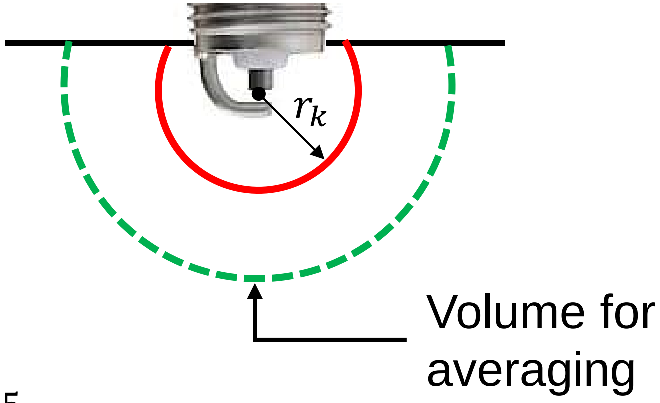
2) **Transport equation**:

$$\frac{\partial \Xi}{\partial t} + \widetilde{\boldsymbol{U}}_s \cdot \nabla \Xi = G\Xi - R(\Xi - 1)$$

$$G = R \frac{\Xi_{eq} - 1}{\Xi_{eq}} \; ; \; R = \frac{0.28}{\tau_{\eta}} \frac{\Xi_{eq}^{*}}{\Xi_{eq}^{*} - 1} ; \Xi_{eq} = 1 + 2\, S_{\Xi} \, (1 - b)\left(\Xi_{eq}^{*} - 1\right)$$

Combustion model

Transition from laminar to turbulent flame propagation



Wrinkle factor during transition: $\Xi = 1 + f\left(\Xi_{eq} - 1\right)$

Transition factor: $f = \left[1 - \exp\left(-\frac{r_k}{\langle L_t \rangle}\right)\right]^{0.5} \cdot \left[1 - exp\left(-\frac{\langle u' \rangle + \langle S_u \rangle}{\langle L_t \rangle} \cdot t_{ign}\right)\right]^{0.5}$

Average flame kernel radius evolution: $\frac{\partial r_k}{\partial t} = \frac{\langle \rho_u \rangle}{\langle \rho_b \rangle} \cdot \langle S \rangle$

Taylor scale to distinguish from laminar to turbulent flame propagation

$$\lambda = \sqrt{10\nu \frac{k}{\varepsilon}}$$

Laminar stretched flame: $r_k < C_{Tay} \cdot \lambda$

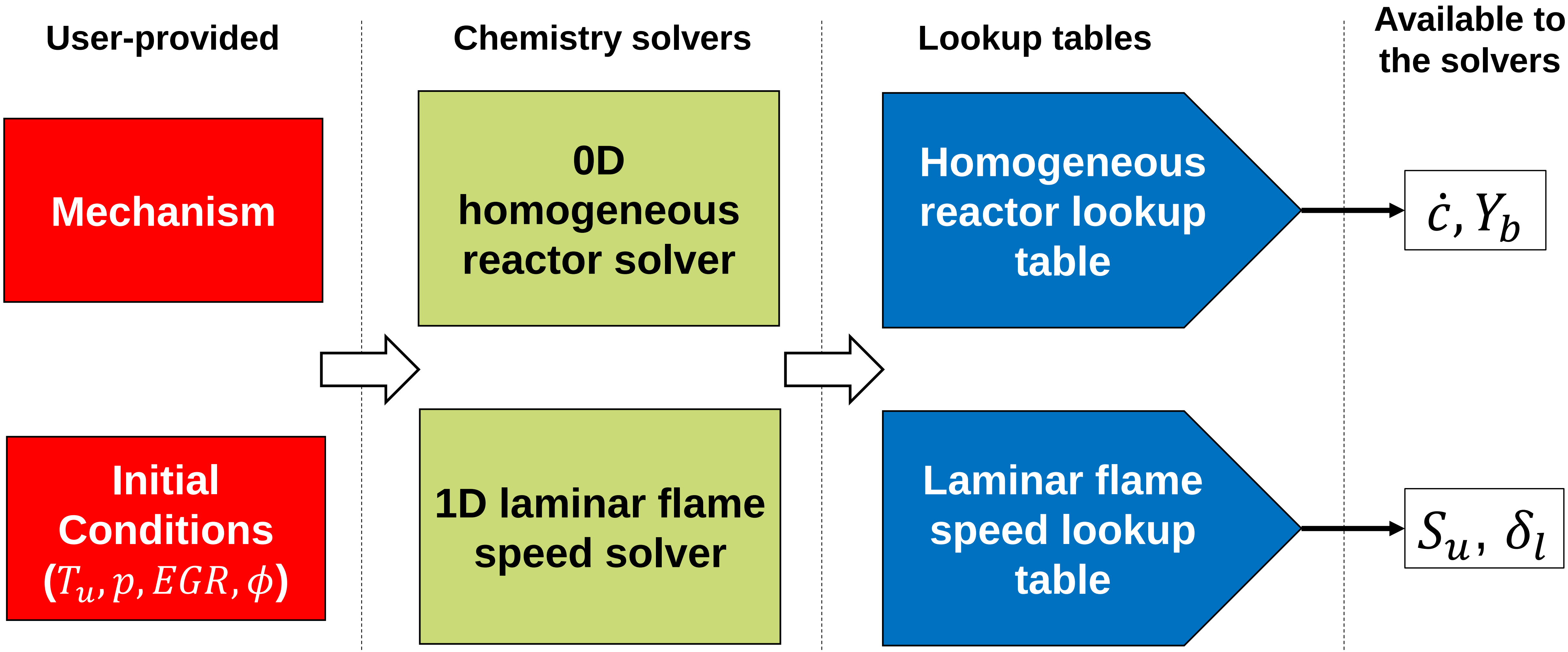
$$S = I_{0L} \cdot S_u \; ; \; I_{0L} = \left(1.0 - \frac{\mathcal{L}_u \kappa}{S_u}\right)$$

Turbulent stretched flame: $r_k > C_{Tay} \cdot \lambda$

$$S = I_{0T} \cdot S_u \cdot f \cdot \Xi_{eq} \; ; I_{0T} = \frac{0.117}{1 + \tau} Ka^{-0.784}$$

Combustion model

Tabulation of detailed kinetics



User-provided

Mechanism

Initial Conditions (T_u, p, EGR, ϕ)

Chemistry solvers

0D homogeneous reactor solver

1D laminar flame speed solver

Lookup tables

Homogeneous reactor lookup table

Laminar flame speed lookup table

Available to the solvers

$\dot{c}, Y_b$

S_u, δ_l

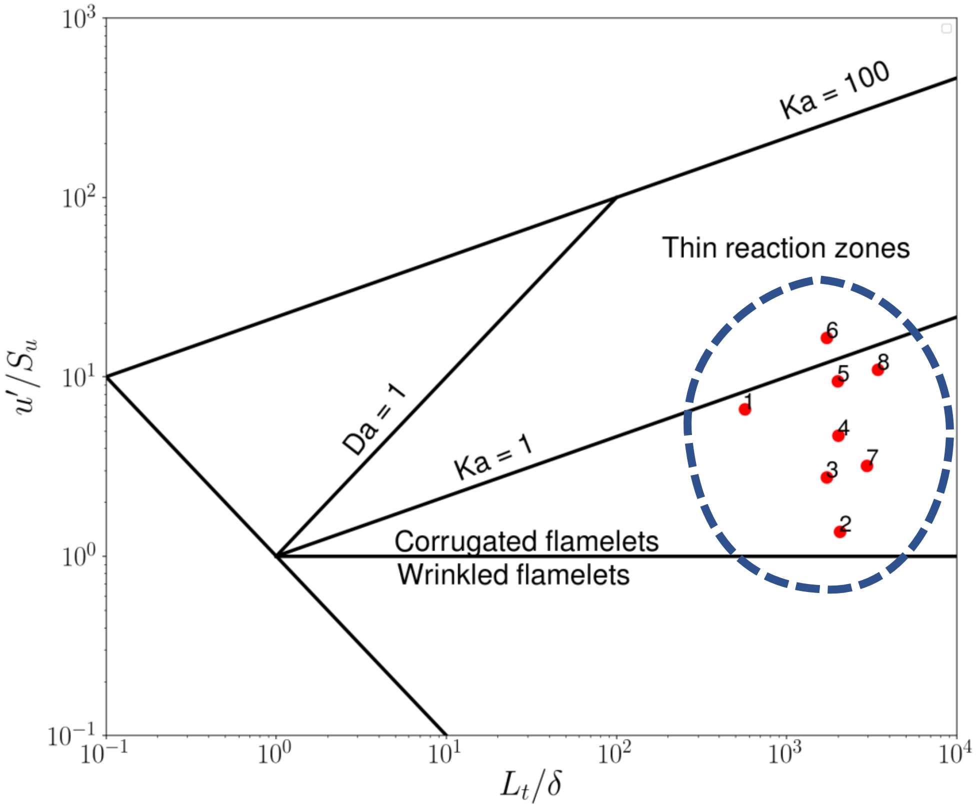
Experimental validation

Constant volume vessel homogeneous combustion validation

M. Lawes, M. P. Ormsby, C.G.W. Sheppard, and R. Woolley. **The turbulent burning velocity of iso-octane/air mixtures.** *Combustion and Flame*, 159(5):1949 – 1959, 2012.

- Extensive database useful for model validation
- Flame radius versus time data available
- Initial vessel temperature: 360 K

Case	u' [m/s]	p [bar]	L_i [mm]	λ [mm]	η [mm]	ϕ	S_u [m/s]	$\mathcal{L}_u$ [mm]
1	1	1	20	2.6	0.120	1	0.51	3.1
2	4	1	20	1.3	0.042	1	0.51	3.1
3	0.5	5	20	1.6	0.060	1	0.30	0.5
4	1	5	20	1.2	0.035	1	0.30	0.5
5	4	5	20	0.6	0.012	1	0.30	0.5
6	6	5	20	0.5	0.009	1	0.30	0.5
7	1	10	20	0.8	0.021	1	0.25	0.2
8	4	10	20	0.4	0.007	1	0.25	0.2

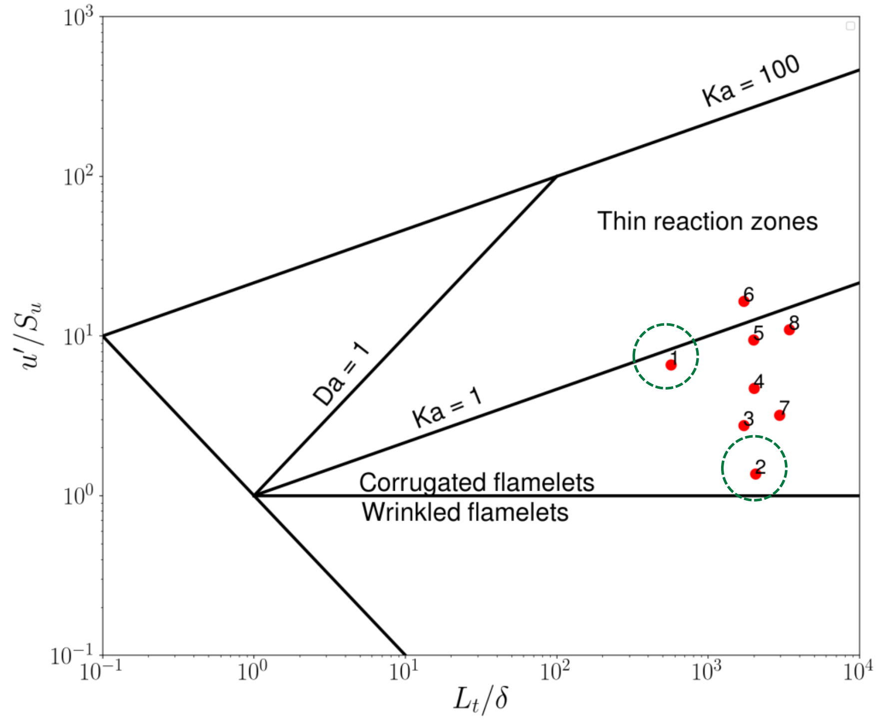


Exp. data in M. Lawes et al., *Comb. Flame*, 2012.

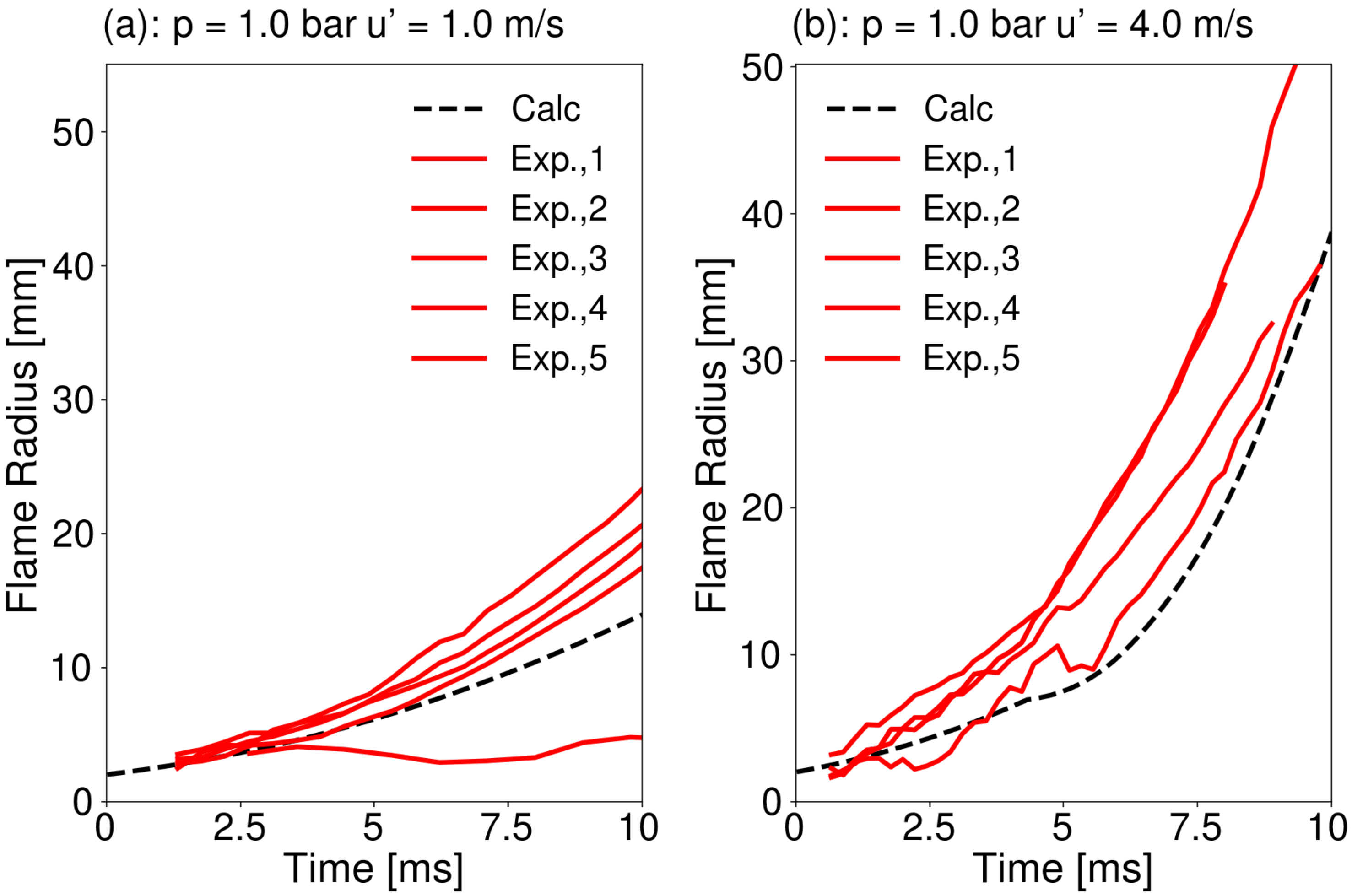
Experimental validation

Constant volume vessel homogeneous combustion validation

Case	u' [m/s]	p [bar]	L_i [mm]	λ [mm]	η [mm]
1	1	1	20	2.6	0.120
2	4	1	20	1.3	0.042



Turbulence intensity effects at p_{amb} = 1 bar


(a): p = 1.0 bar u' = 1.0 m/s

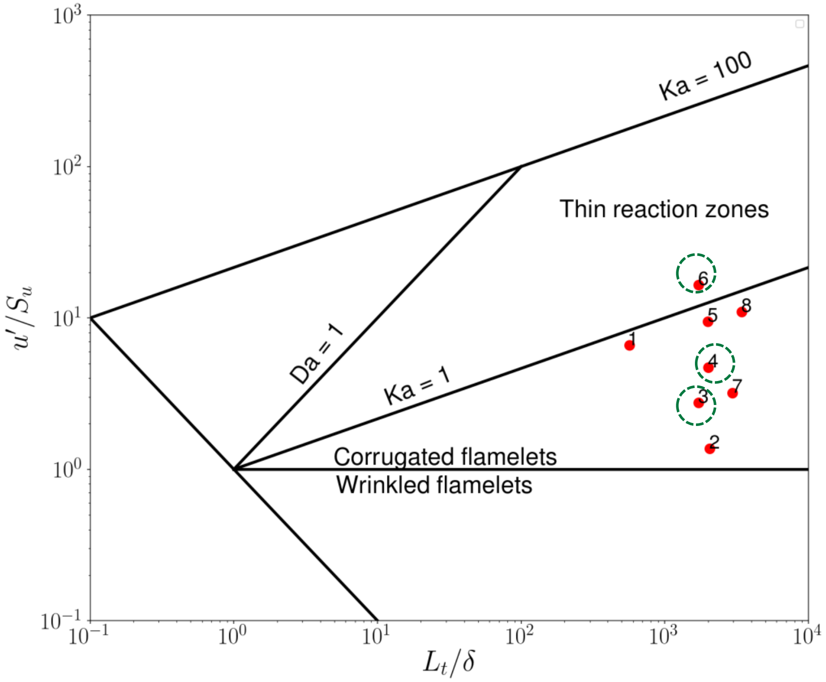
(b): p = 1.0 bar u' = 4.0 m/s

Experimental validation

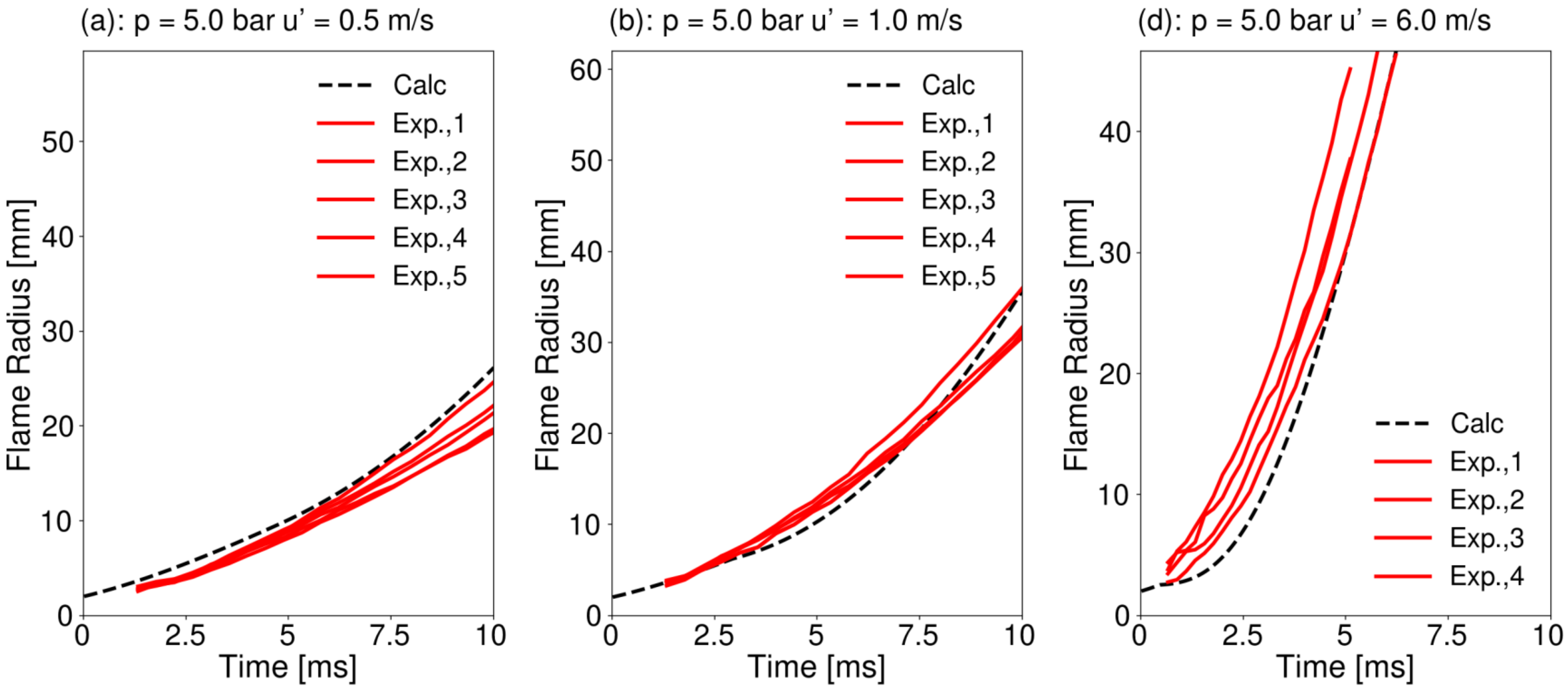
Exp. data in M. Lawes et al., *Comb. Flame*, 2012.

Constant volume vessel homogeneous combustion validation

Case	u' [m/s]	p [bar]	L_i [mm]	λ [mm]	η [mm]
3	0.5	5	20	1.6	0.060
4	1	5	20	1.2	0.035
6	6	5	20	0.5	0.009



Turbulence intensity effects at p_{amb} = 5 bar



Simulations show that increase of turbulence intensity produces:

- Reduced duration of the laminar to turbulent transition phase
- Increased flame speed

Experimental validation

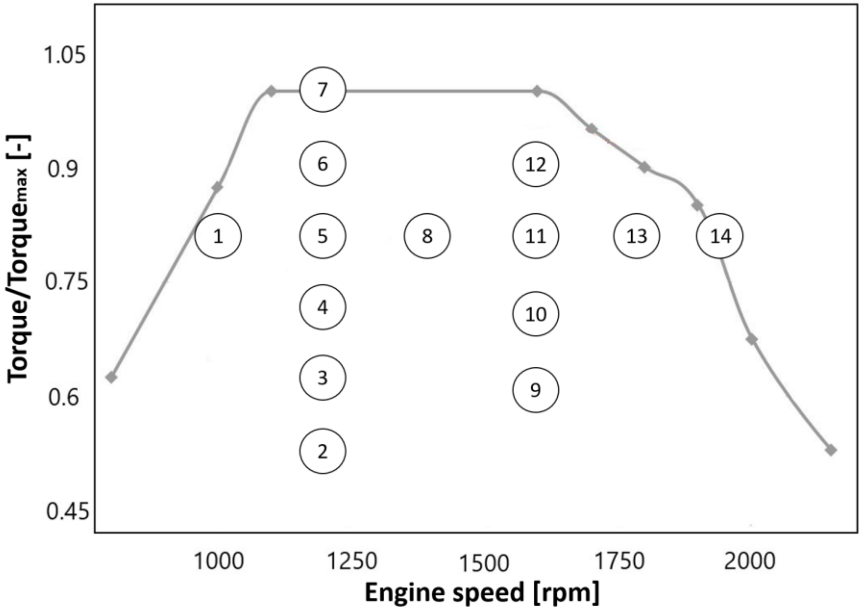
Heavy-duty natural gas engine

Main engine data

Bore [mm]	135
Stroke [mm]	150
CR	≈12
IVC [CAD ATDC]	-175
EVO [CAD ATDC]	124
Swirl	≈1.5

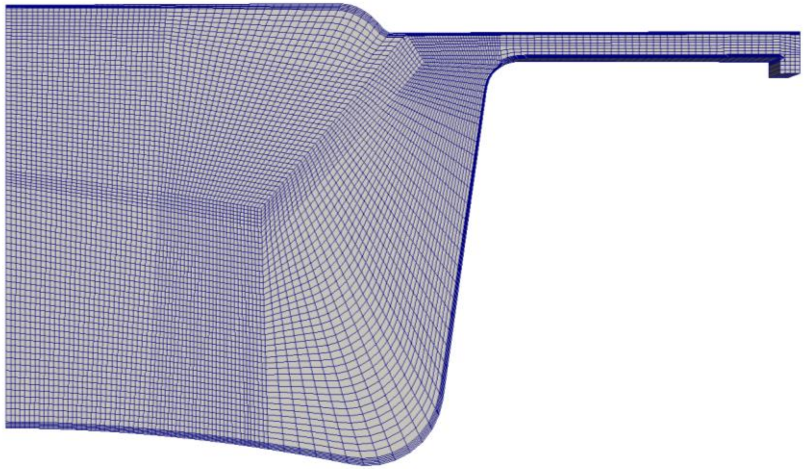
- IVC conditions (p, T, residuals): from 1D engine simulations
- Swirl number: from full-cycle simulations of the gas exchange process

Simulated operating points



- 14 conditions, variation of engine load and speed

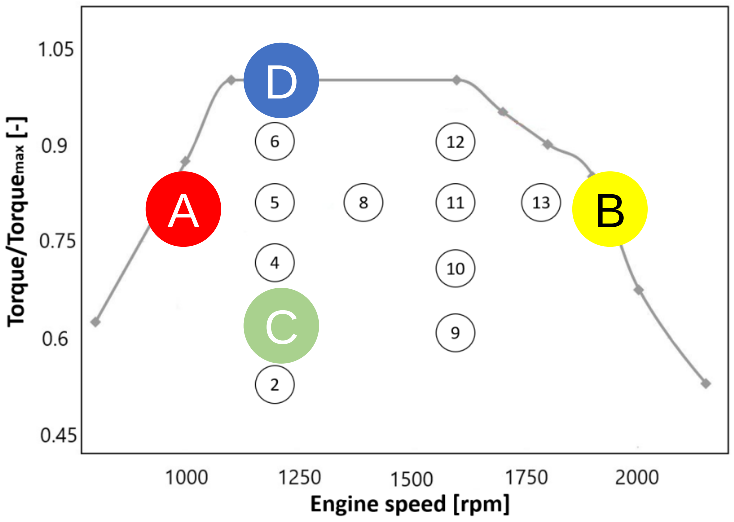
Mesh and case setup

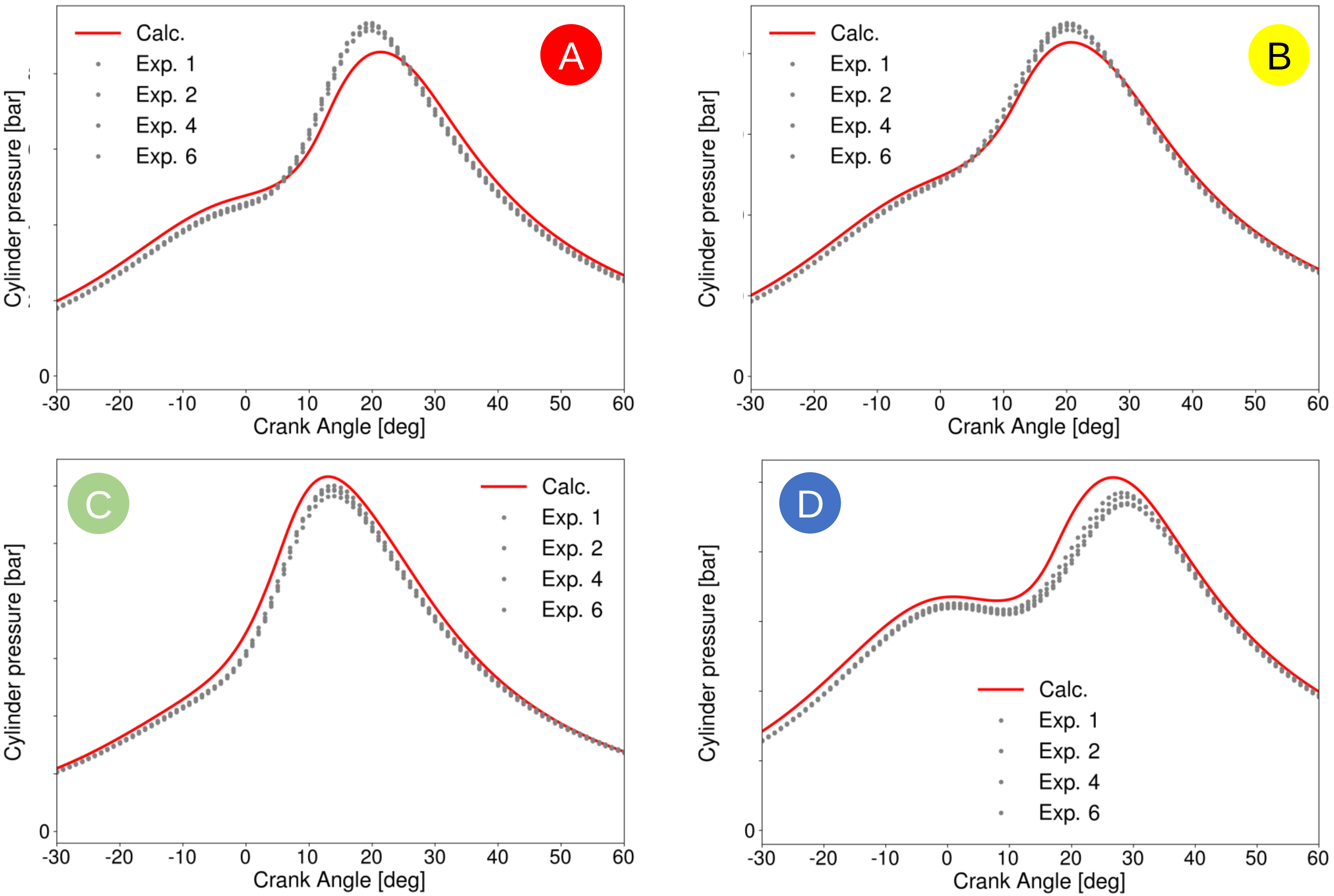


- Computational mesh generated with the python Polimi graphical interface for automatic mesh generation

Experimental validation

Heavy-duty natural gas engine





- Algebraic expression for the wrinkle factor:

$$\Xi = 1 + f\,(\Xi_{eq} - 1)$$

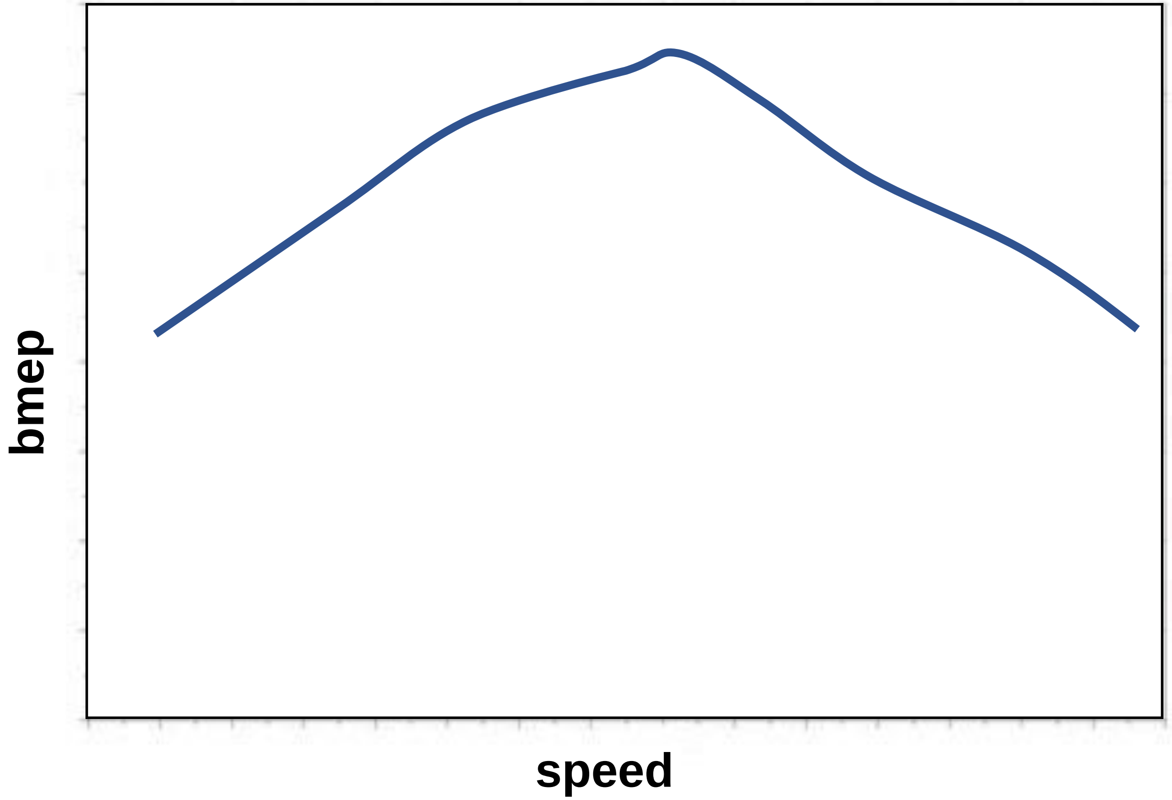
- Experimental values of the spark advance used in all the simulations
- No variation in model tuning coefficients

Acknowledgments: P. Soltic, C. Bach (EMPA)

Experimental validation

Light-duty natural gas engine

Engine geometry data		
Displaced volume	3.0	[dm³]
Bore	96	[mm]
Stroke	105	[mm]
Compression ratio	≈ 12	[-]
Number of valves	4	[-]



Large database of operating conditions to study the combustion process:

- **<u>baseline</u>**
- modified intake system
- modified piston bowl geometries

Mesh influence:

- 2D mesh with imposed flow field at IVC
- Full-cycle simulation in a 3D mesh

Combustion model study:

- Algebraic vs Two-Equation Weller model

Experimental validation

Light-duty natural gas engine

Automatic mesh generation for 3D combustion chambers (SI engines)

Background mesh

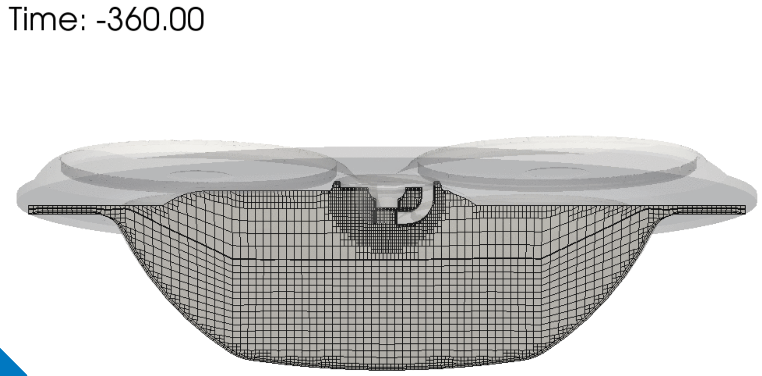
Automatically generated from the main engine geometry data

Mean cell size	0.7 [mm]

Combustion chamber mesh

From combustion chamber geometry (triangulated surface format) and background mesh using `snappyHexMesh`

Min. number of cells (TDC)	430’000



Moving mesh (using layer addition and removal): combustion simulations performed with a single mesh.

Max. number of cells (BDC)	970’000

Experimental validation

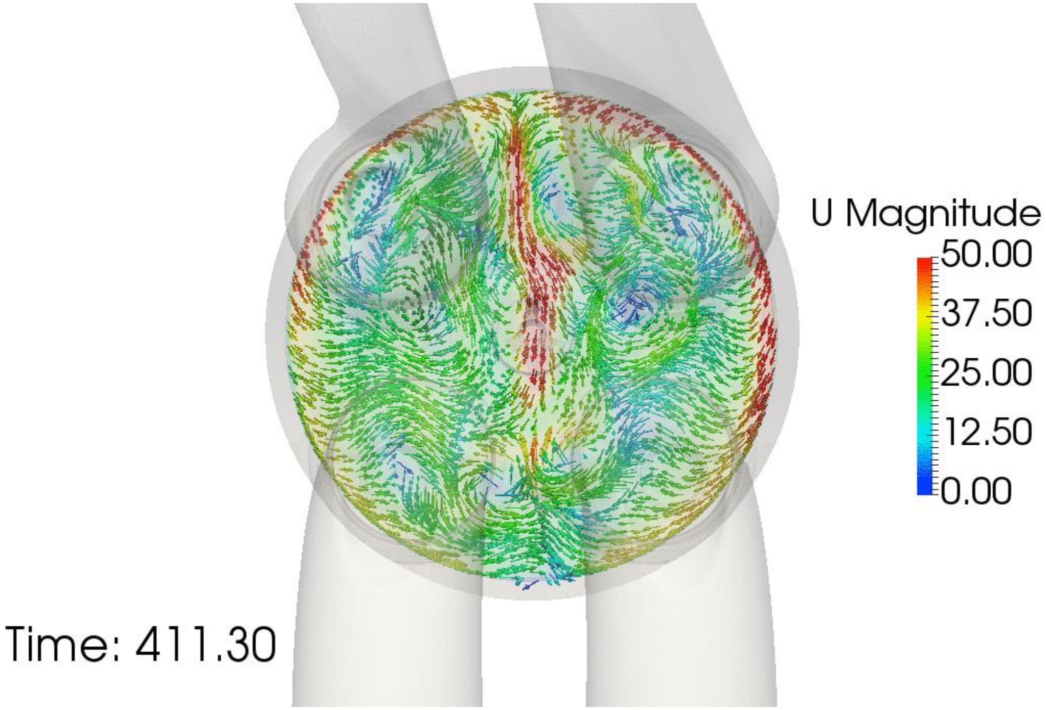
Acknowledgments: P. Soltic, C. Bach (EMPA)

Light-duty natural gas engine

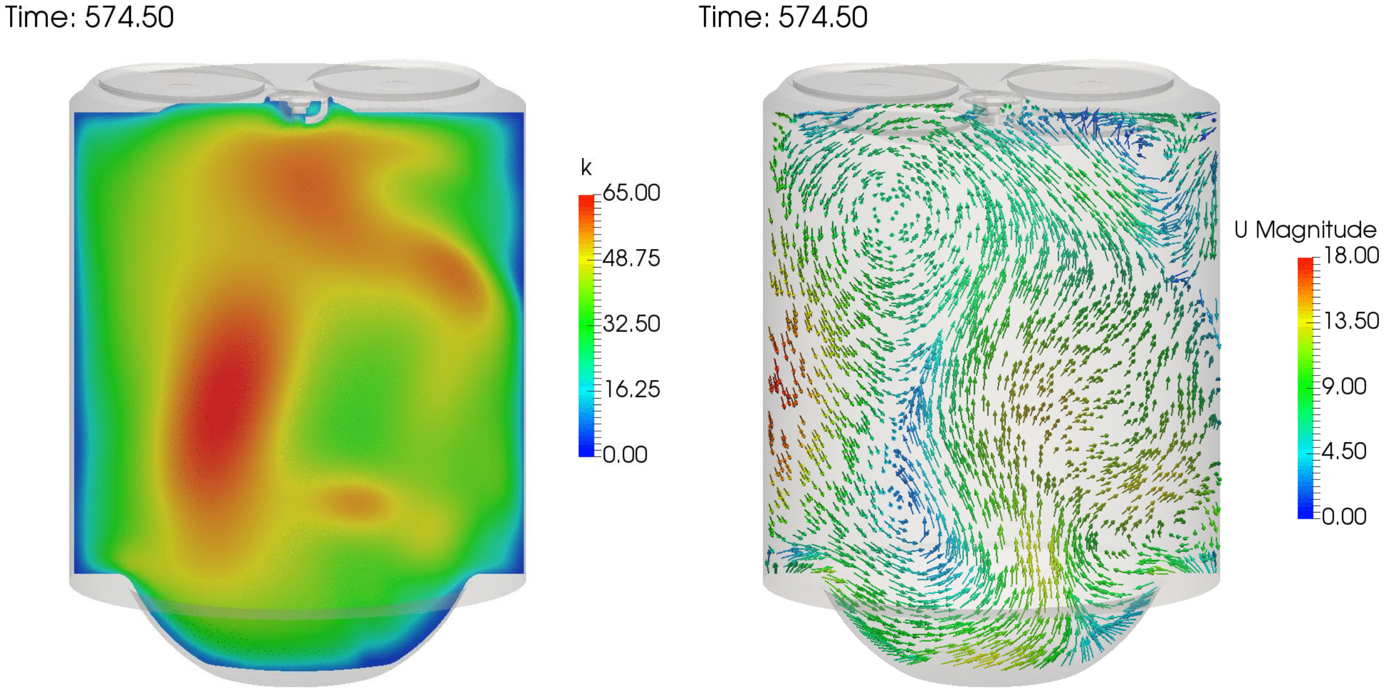
3D mesh: flow field from full-cycle simulation

Intake process and charge motion development

In-cylinder turbulence and flow during compression stroke



Almost symmetric swirl flow at spark advance



Non-uniform turbulence distribution + “secondary flows”

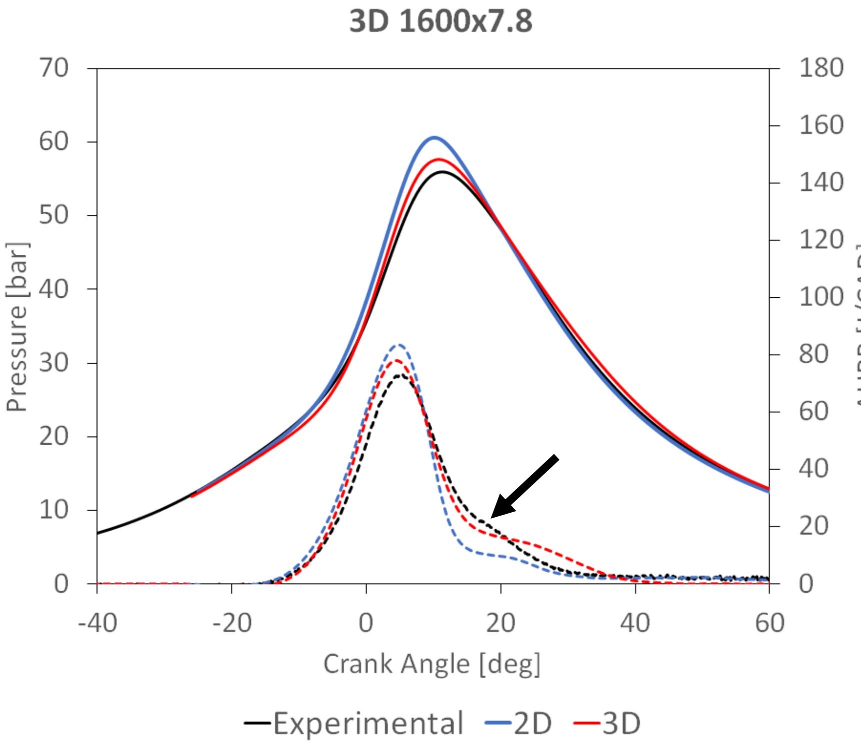
Experimental validation

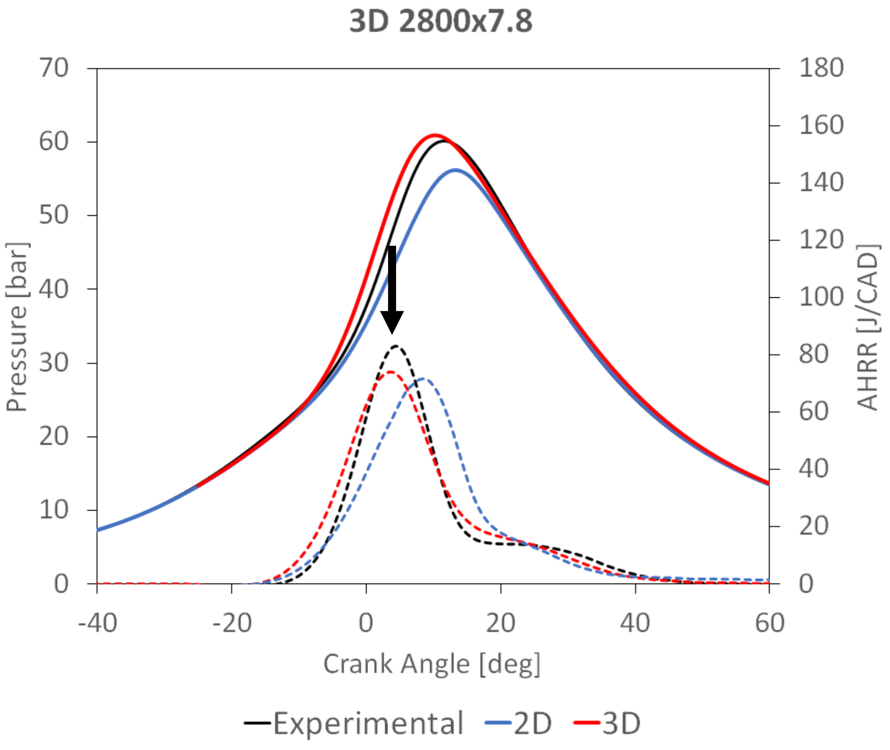
Light-duty natural gas engine

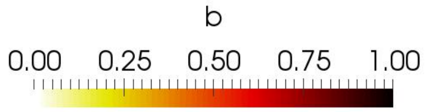
Acknowledgments: P. Soltic, C. Bach (EMPA)

2D vs 3D mesh: combustion process

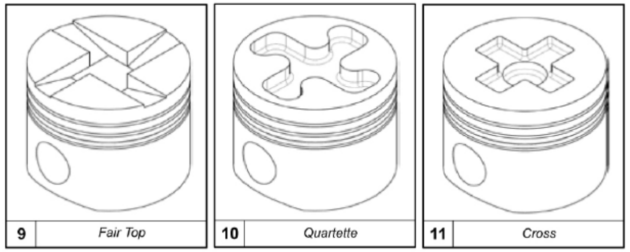
- Better capability to reproduce cylinder pressure and heat release rate at different speeds







Next steps: piston bowl geometry effects on combustion efficiency



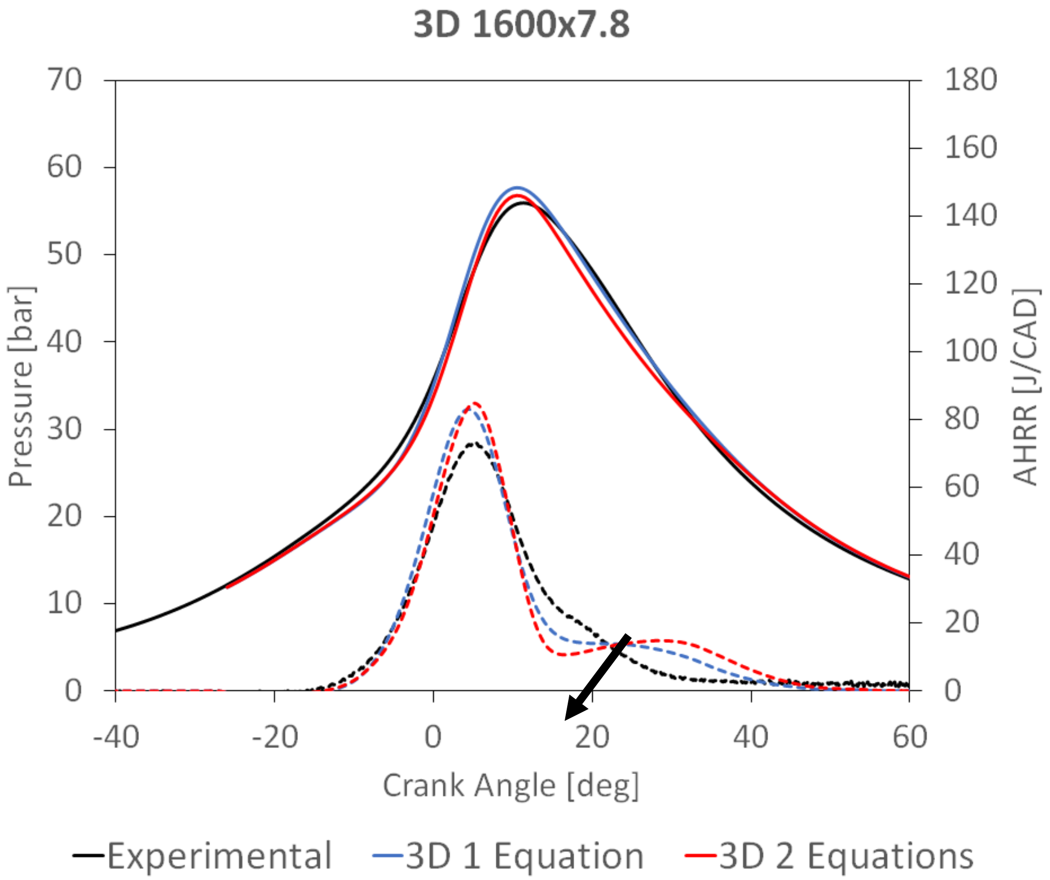
From SAE 2014-01-1326

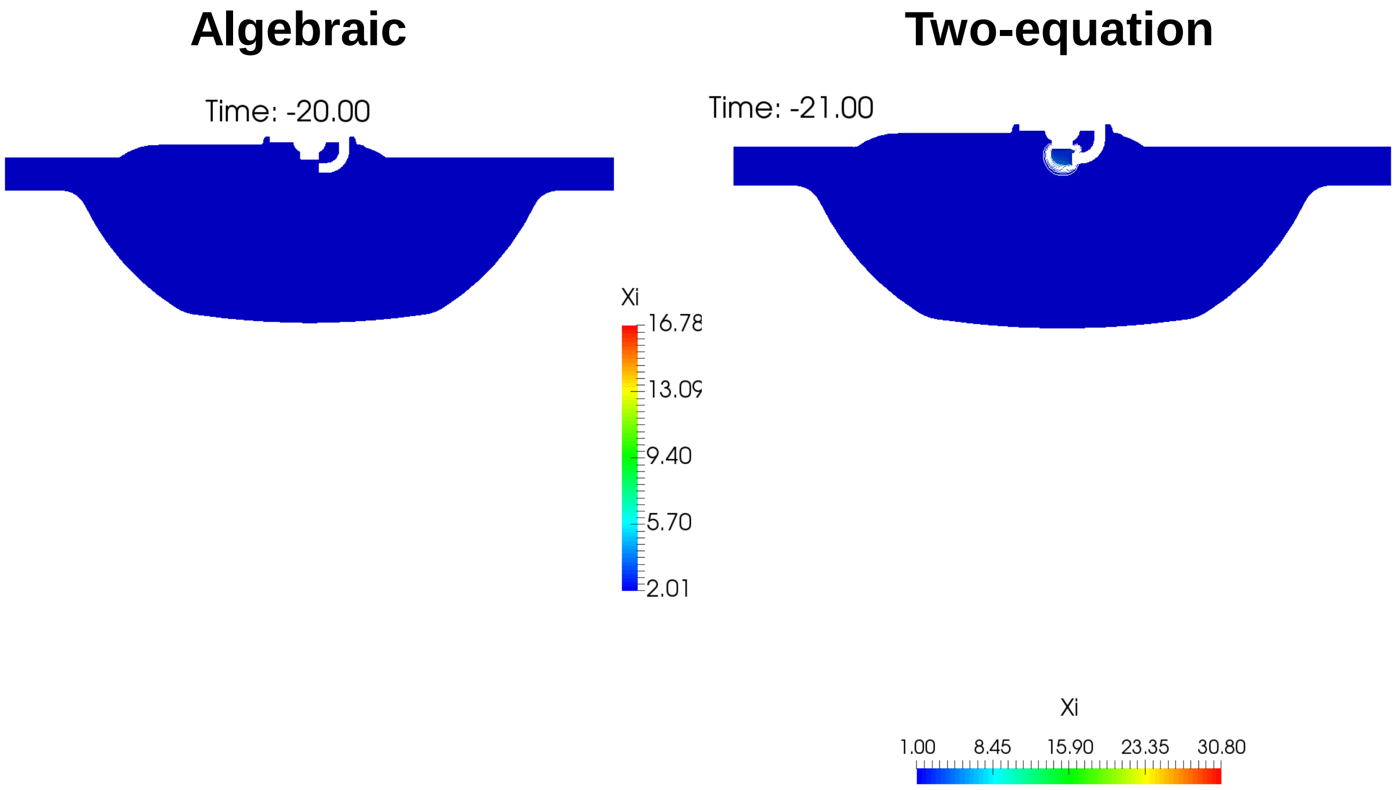
Acknowledgments: P. Soltic, C. Bach (EMPA)

Experimental validation

Light-duty natural gas engine

Algebraic vs Two-Equation model


3D 1600x7.8


Algebraic

Two-equation

- Two-equation model capable to reproduce the combustion process
- Different estimation of the heat release rate towards the end of combustion: two equation model more sensitive to local flow conditions
- Flame wrinkle factor grows across the flame.

Experimental validation

Acknowledgments: M. Bardi, X. Gautrot (IFPEn),
Upgrade EU Project

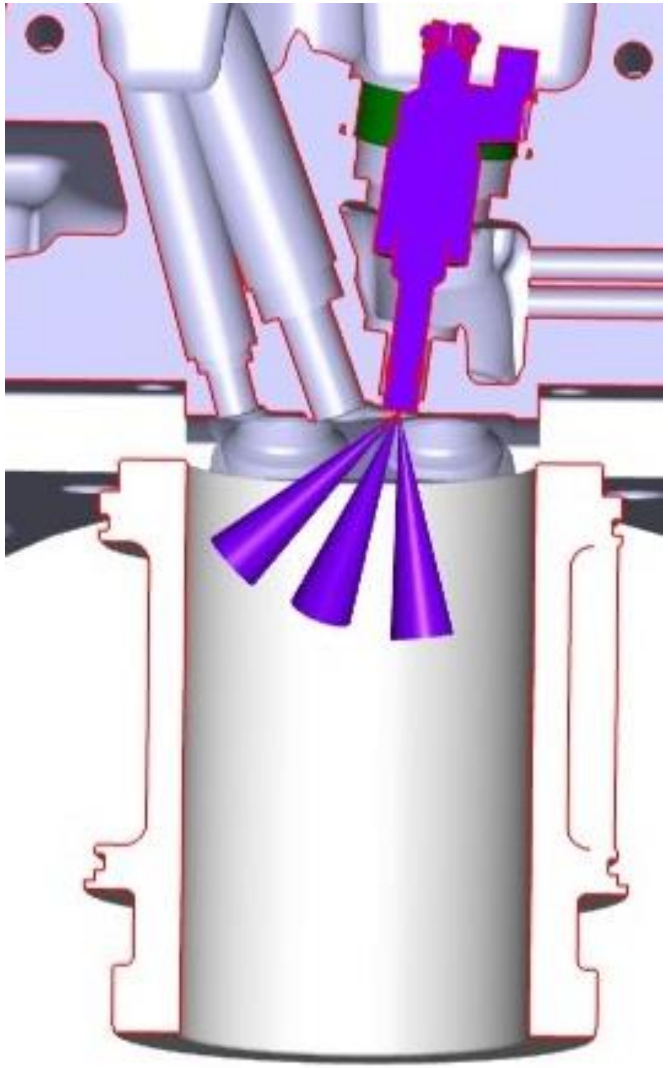
Optically accessible gasoline direct-injection engine

Main engine data

Bore [mm]	77
Stroke [mm]	85.8
Connecting rod lenght [mm]	144
IVO/IVC [CAD ATDC]	360/573
EVO/EVC [CAD ATDC]	129/361
Speed [rpm]	1200
imep [bar]	4.5

Optical measurements

- Flame chemiluminescence
- Soot incandescence
- Spray shadowgraphy



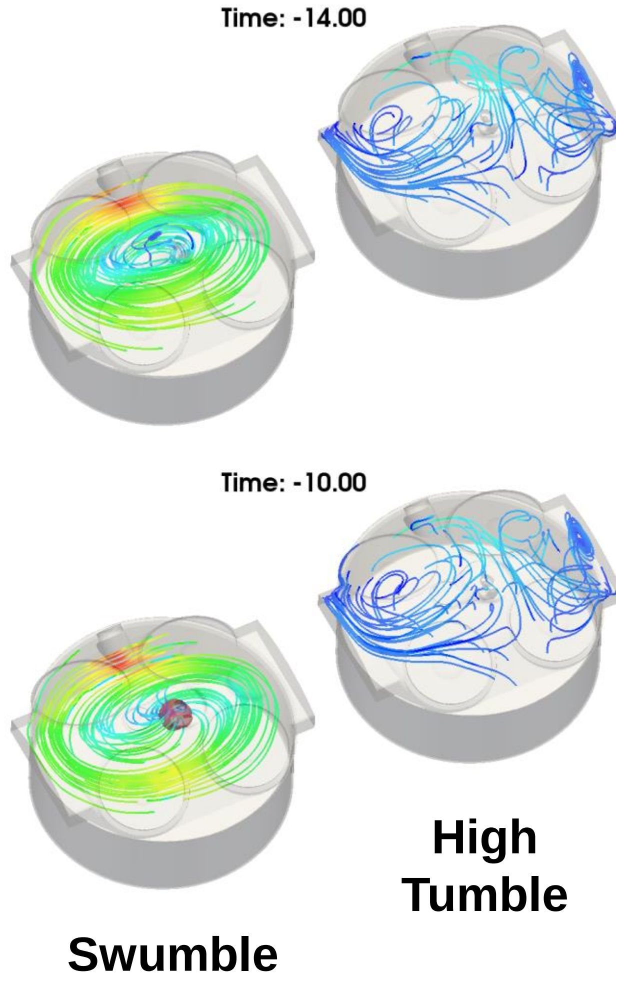
Simulations: effects of in-cylinder charge motions on combustion.

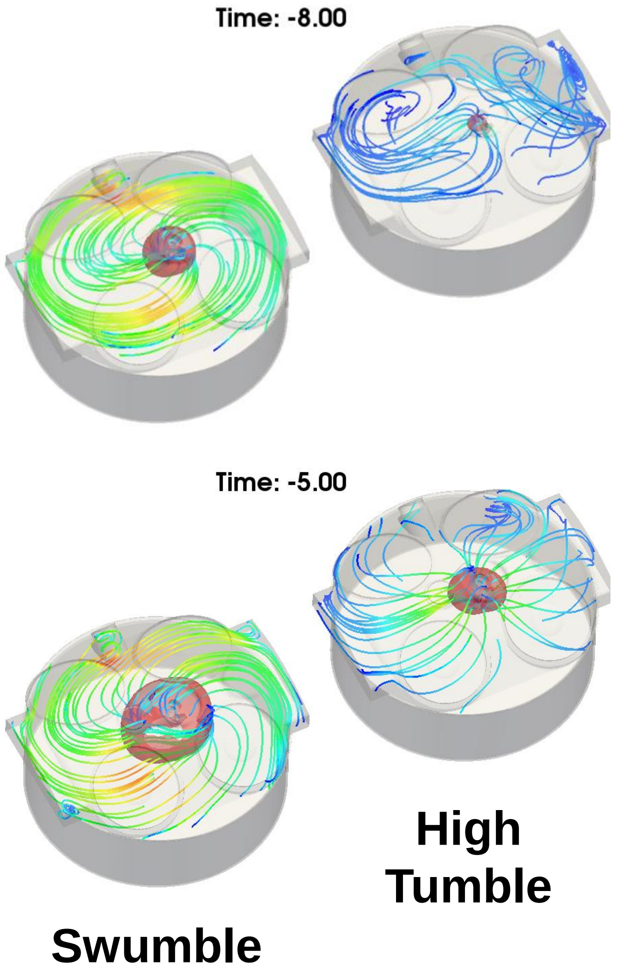
Swumble **Tumble**

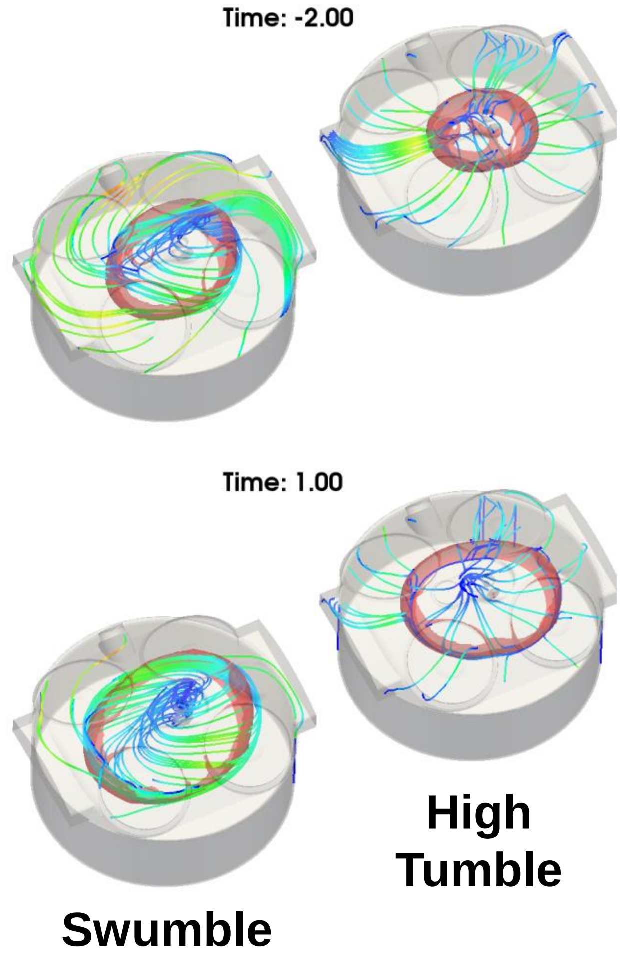
Experimental validation

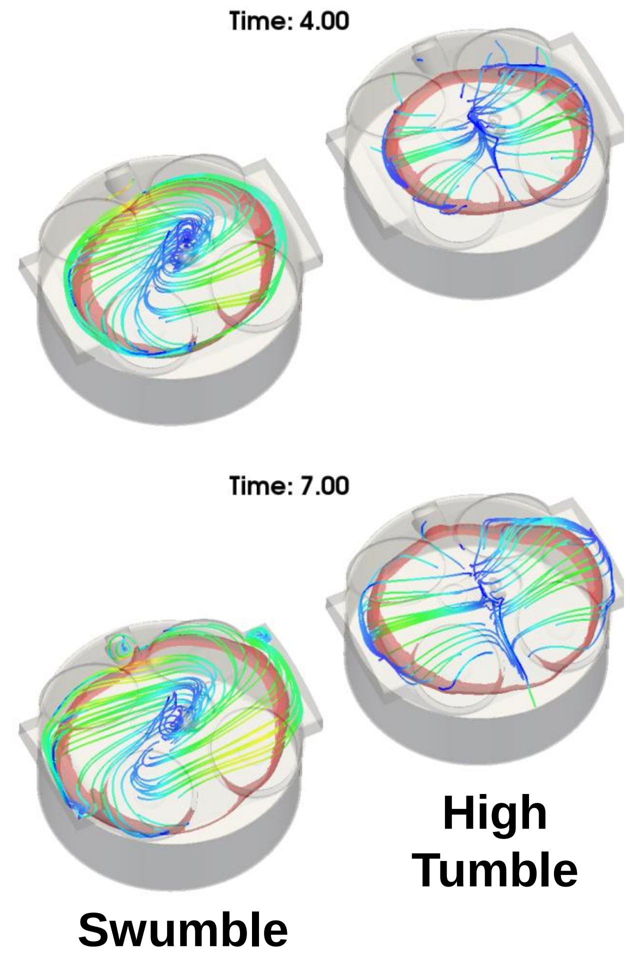
Acknowledgments: M. Bardi, X. Gautrot (IFPEn),
Upgrade EU Project

Optically accessible gasoline direct-injection engine









Experimental validation

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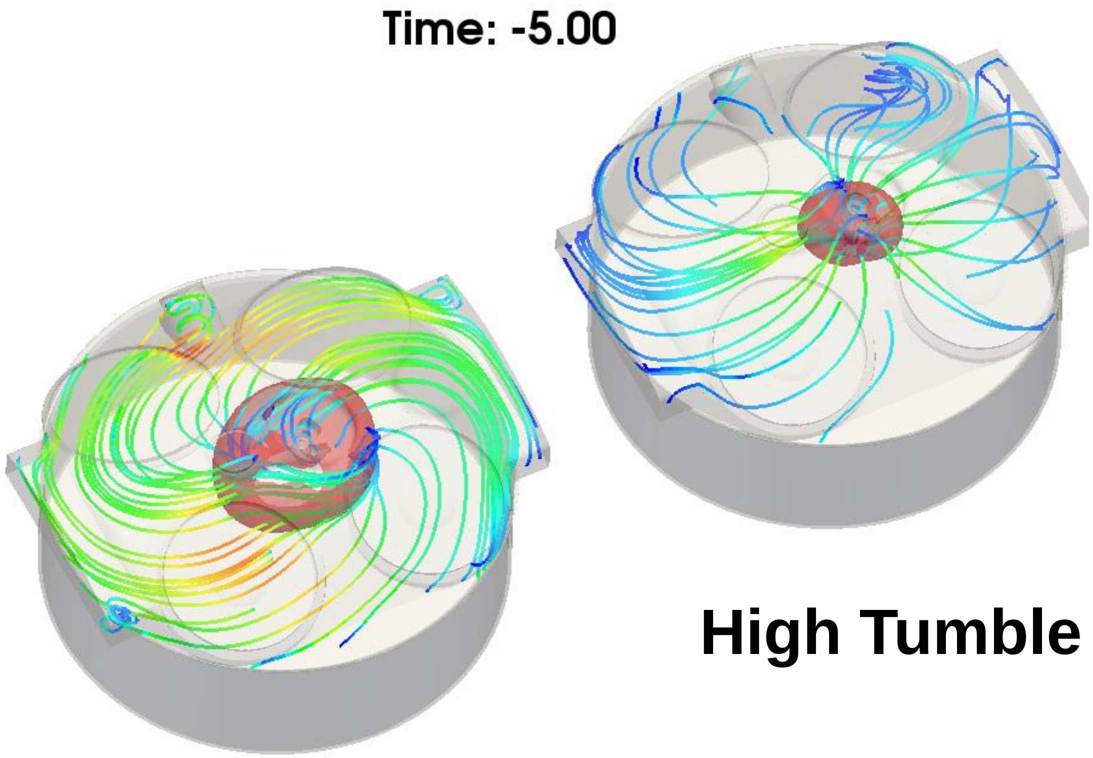
Upgrade EU Project

Optically accessible gasoline direct-injection engine

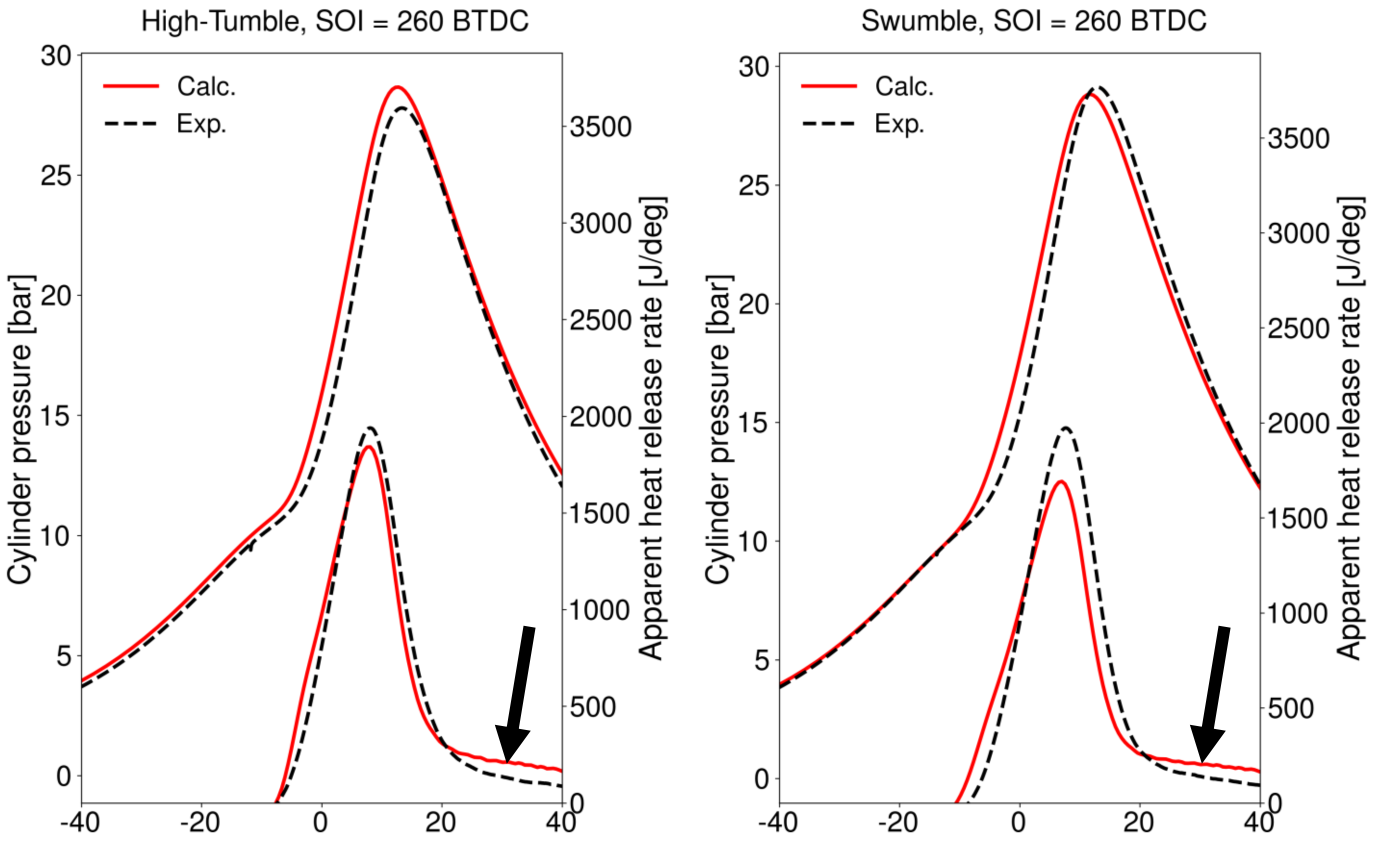


High Tumble

Swumble

Swamble motion persisting during and after combustion
No tumble motion found already at spark-timing

Cylinder pressure and heat release rate validation

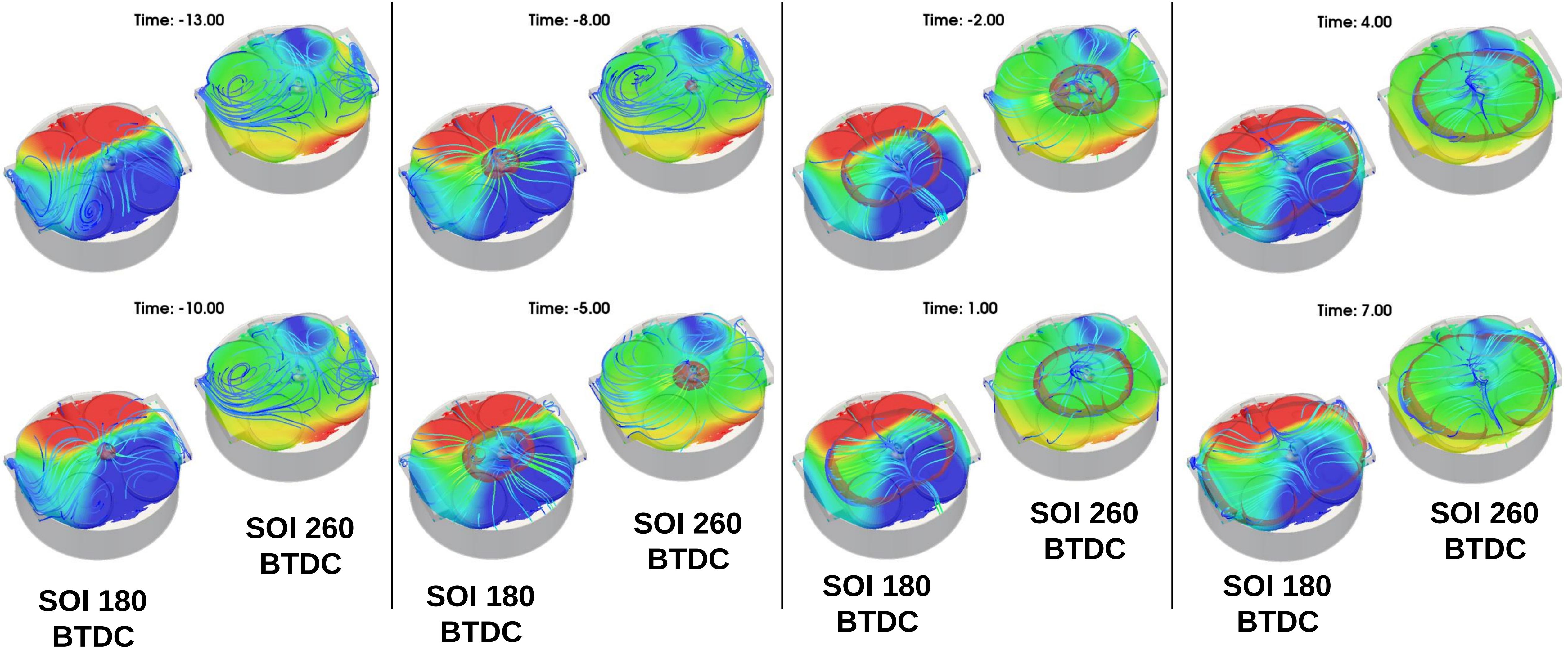


- Rather good match between compute and exp. cyl. pressure
- Deep crevices affecting the burnout phase

Experimental validation

Acknowledgments: M. Bardi, X. Gautrot (IFPEn),
Upgrade EU Project

Optically accessible gasoline direct-injection engine

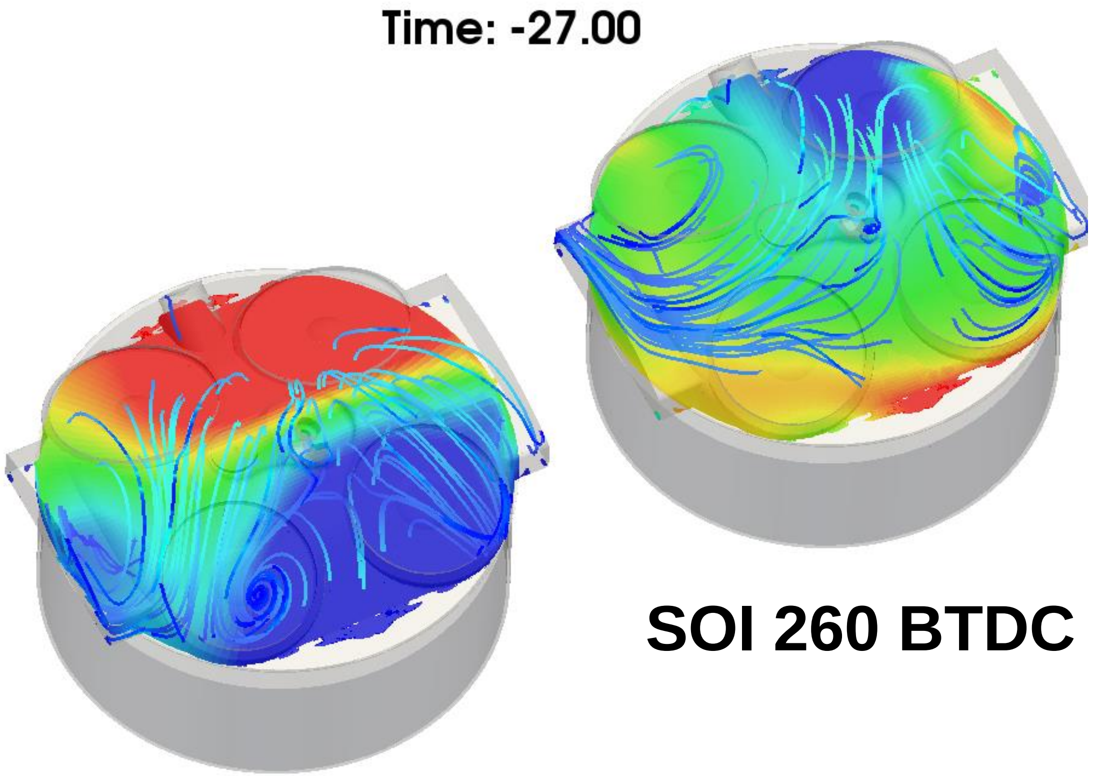


Mixture fraction distribution reported in the cut-plane

Experimental validation

Acknowledgments: M. Bardi, X. Gautrot (IFPEn),
Upgrade EU Project

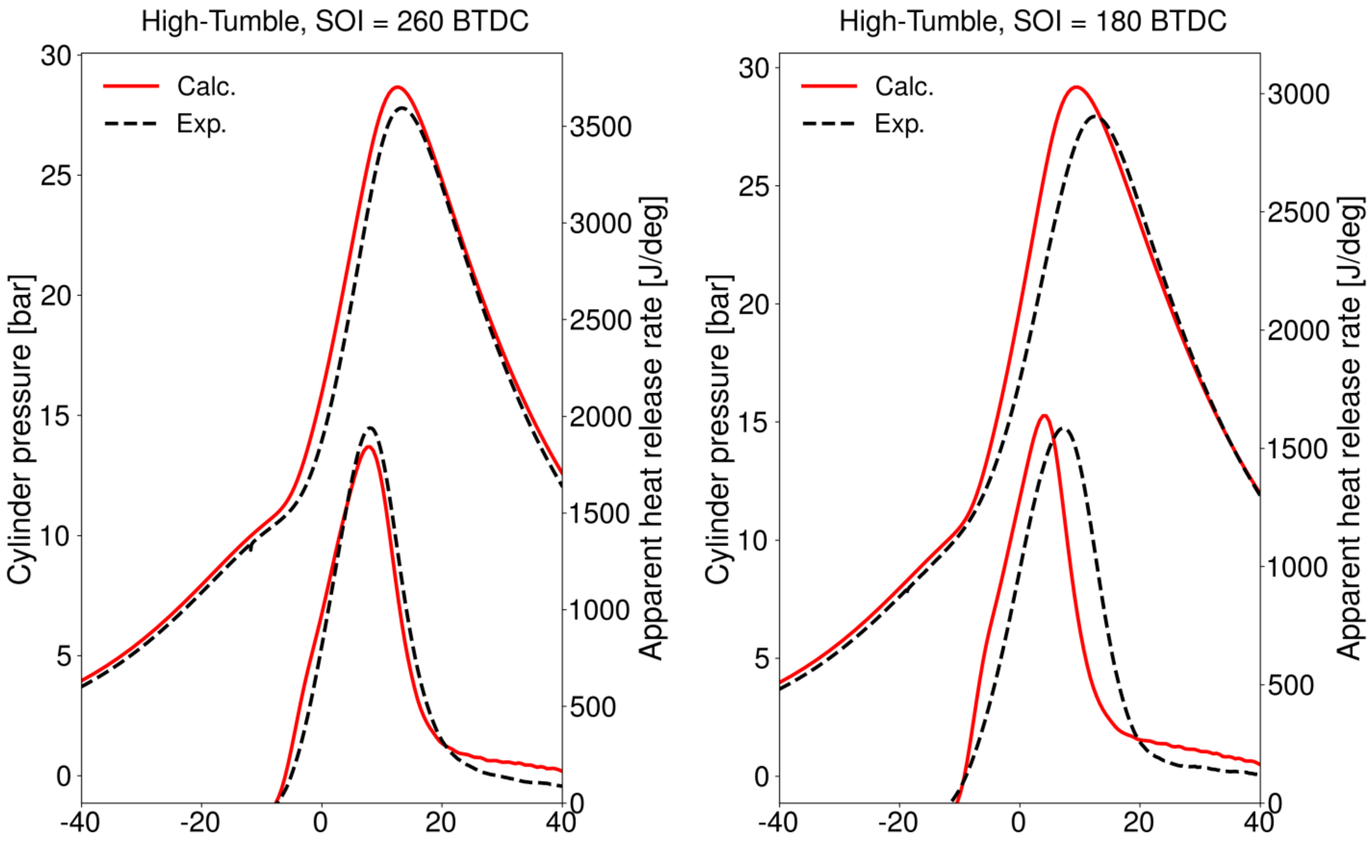
Optically accessible gasoline direct-injection engine



SOI 260 BTDC

SOI 180 BTDC

Cylinder pressure and heat release rate validation

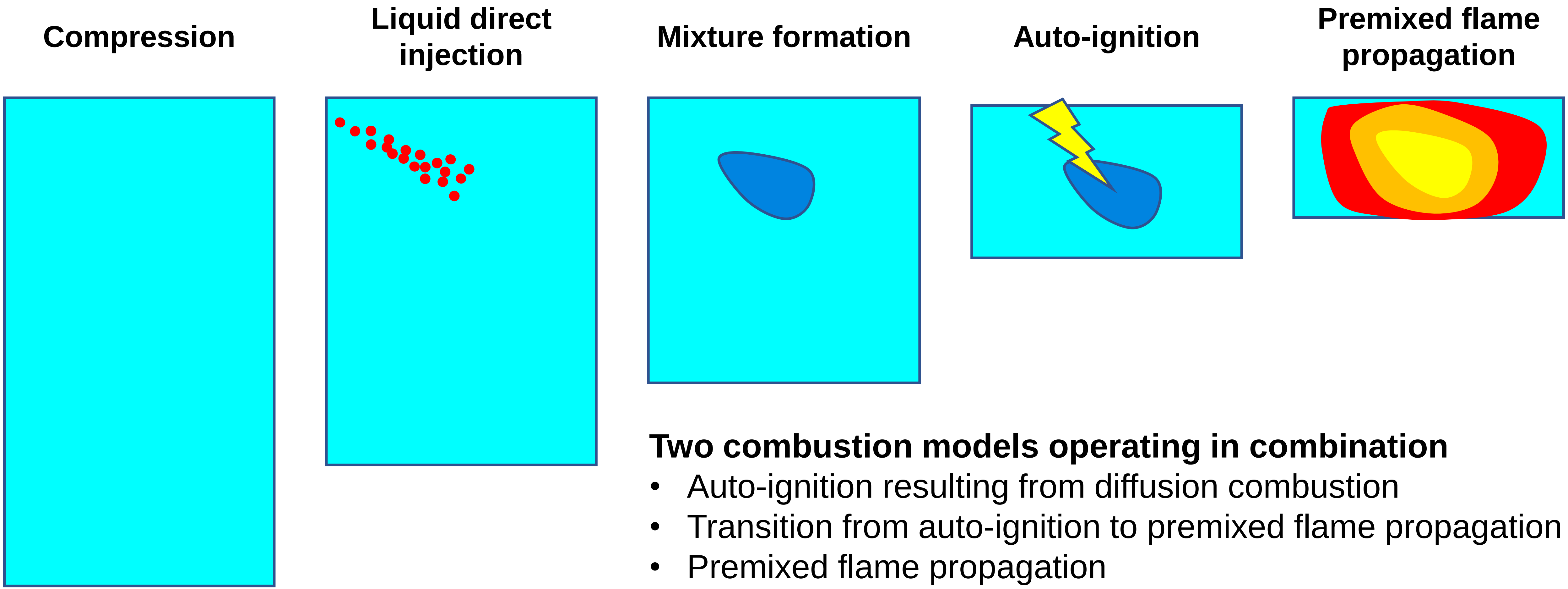


Mixture fraction distribution reported in the cut-plane
Increased charge inhomogeneities due to the delayed SOI.

Advanced concepts

Dual-fuel combustion

Power-cycle phases and needed modeling



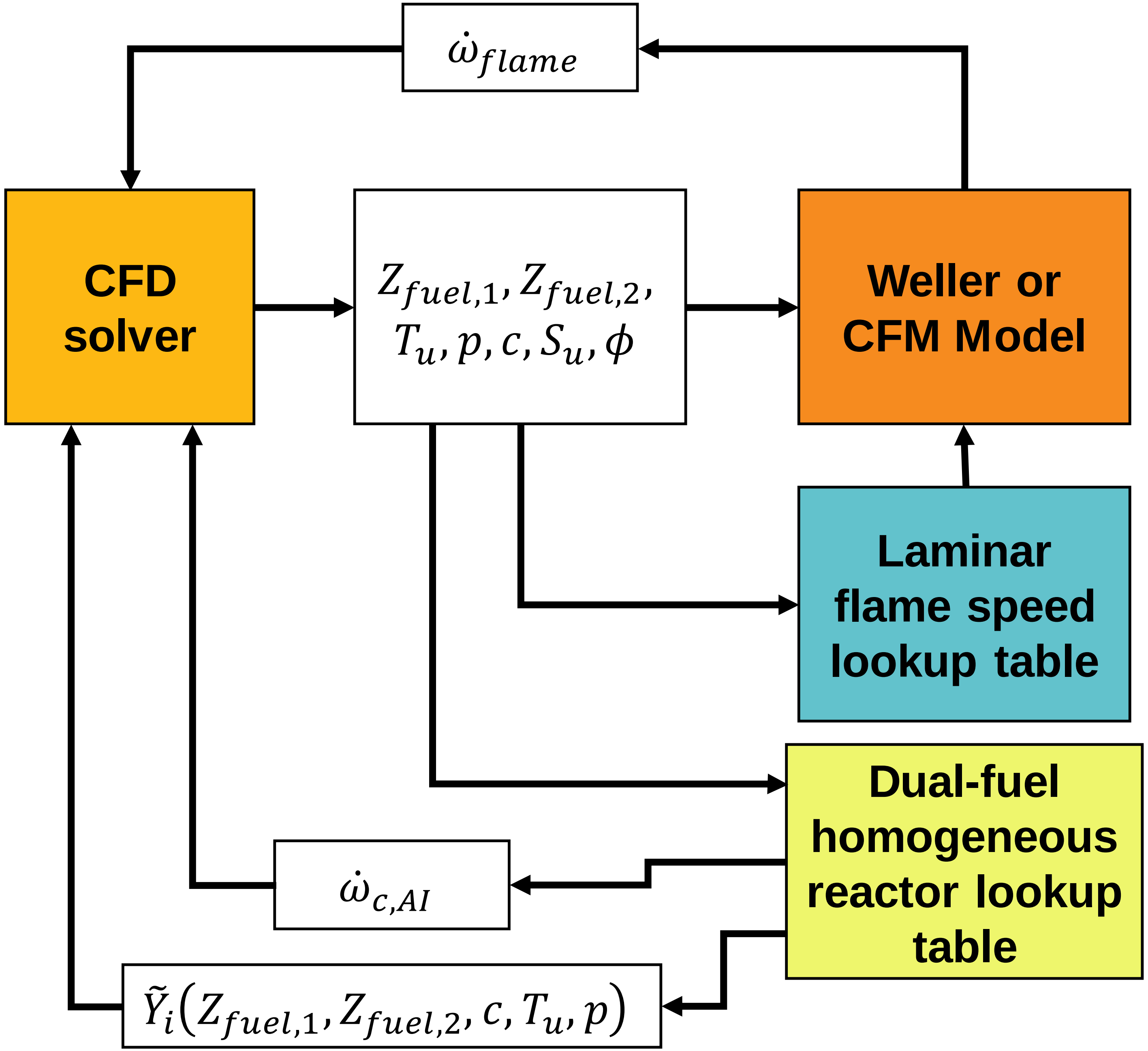
Two combustion models operating in combination

- Auto-ignition resulting from diffusion combustion
- Transition from auto-ignition to premixed flame propagation
- Premixed flame propagation

Dual-fuel combustion

Modeling

- Two transport equations for “premixed” and “diffusive” fuel mixture fractions
- Weller or CFM models for premixed combustion
- Dual-fuel homogeneous reactor lookup table to estimate reaction rate during the auto-ignition mode.
- Progress variable reaction rate accounting for either auto-ignition or flame propagation reation rate
- Premixed combustion model is activated when:
  - progress variable overcomes a user specified value $c > c_{trans}$ and
  - burned mass fraction is higher than a threshold value $x_b > x_{b,trans}$



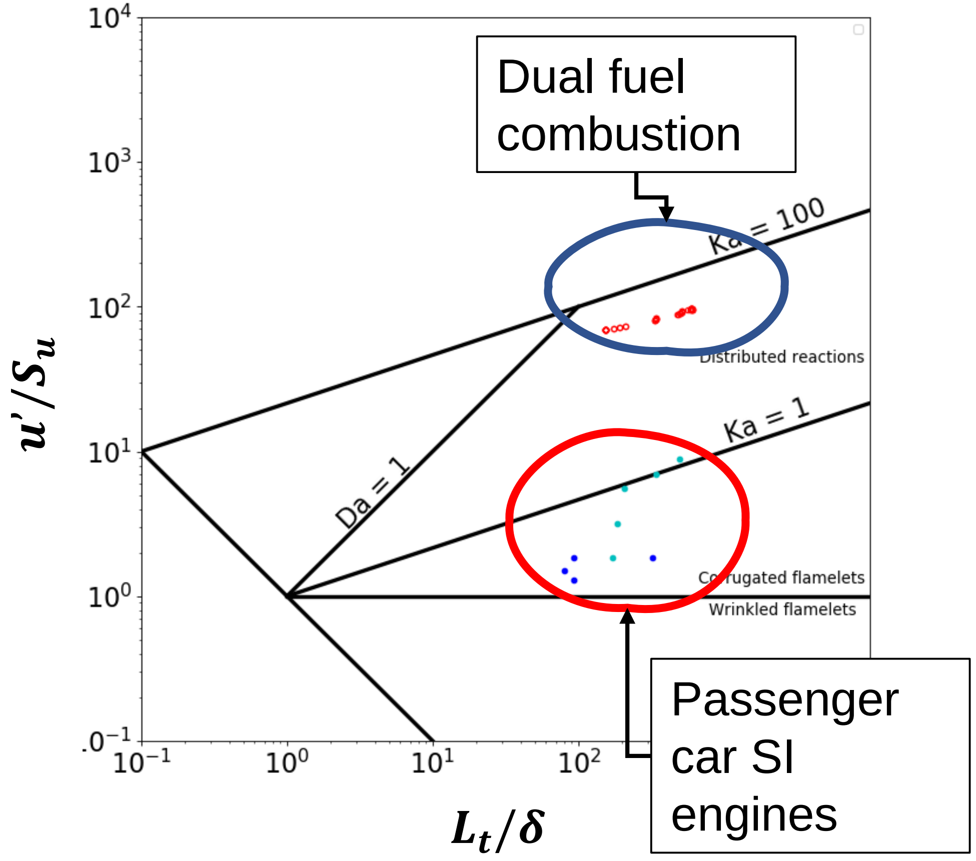
Dual-fuel combustion

Validation on Heavy-Duty engine

Acknowledgments: E. Lendormy (Wartsila)

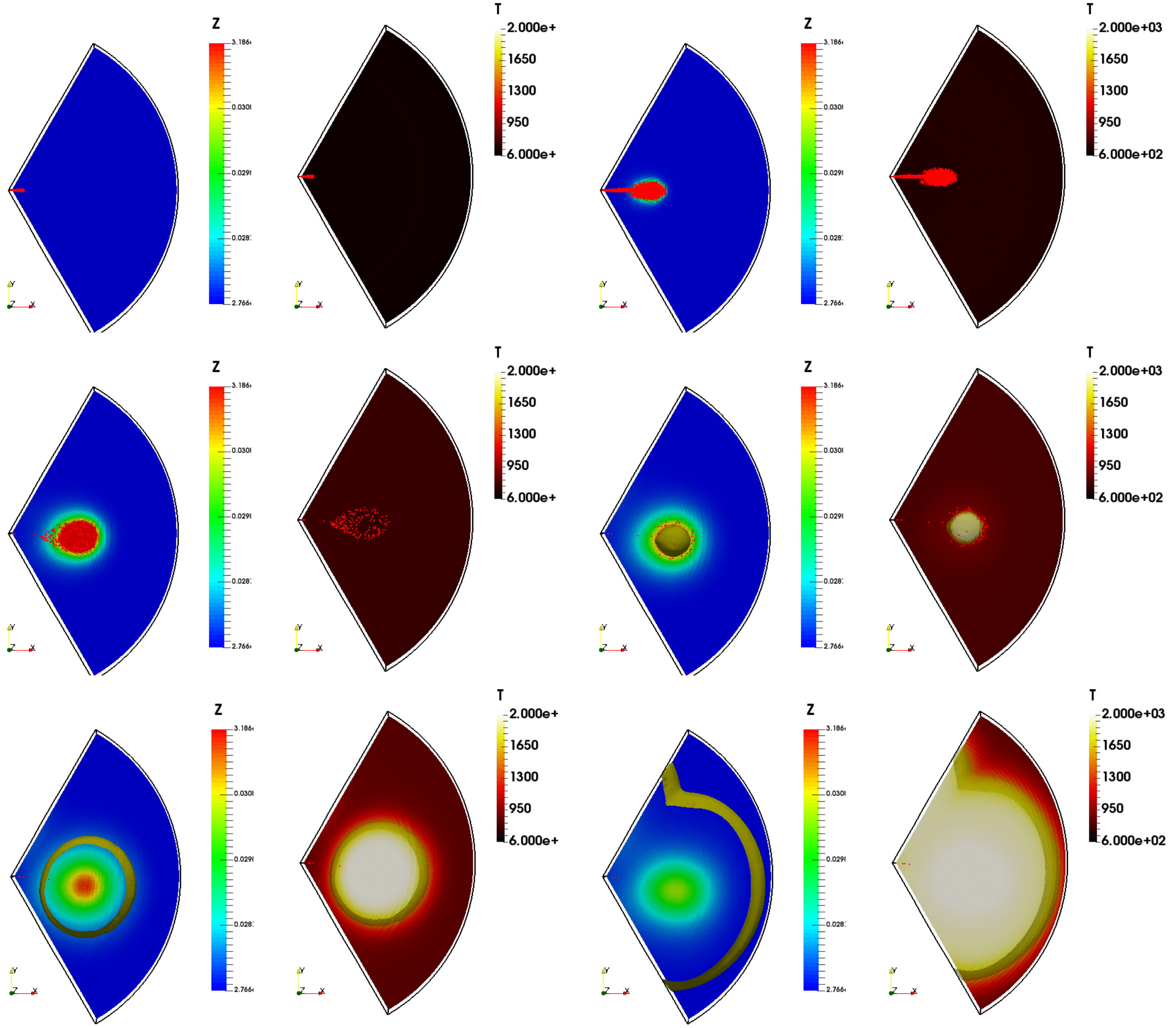
Injection, mixture formation, auto-ignition and premixed flame propagation

- $\phi_{premixed} = 0.5$ + Diesel pilot injection
- Combustion expected to take place at high Karlovitz numbers



Dual fuel combustion

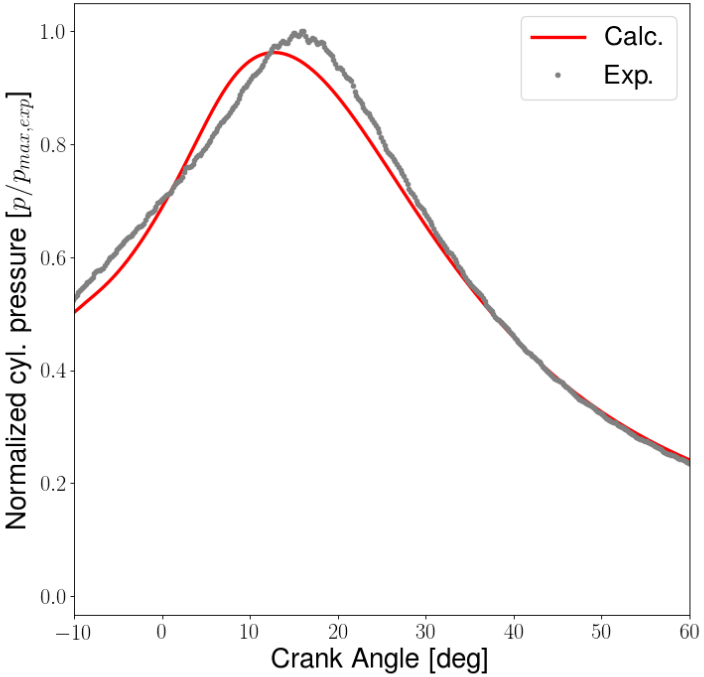
Passenger car SI engines



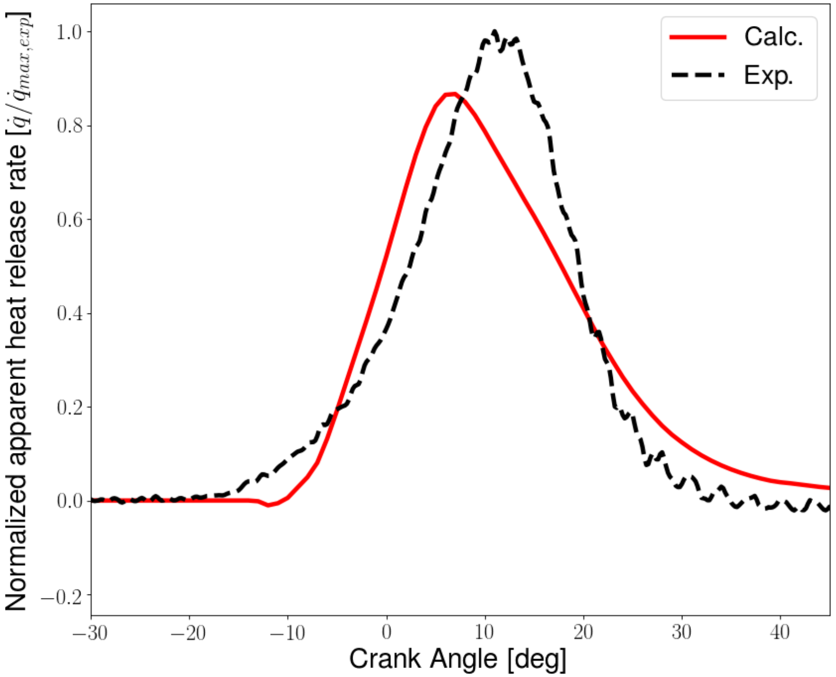
Acknowledgments: E. Lendormy (Wartsila)

Dual-fuel combustion

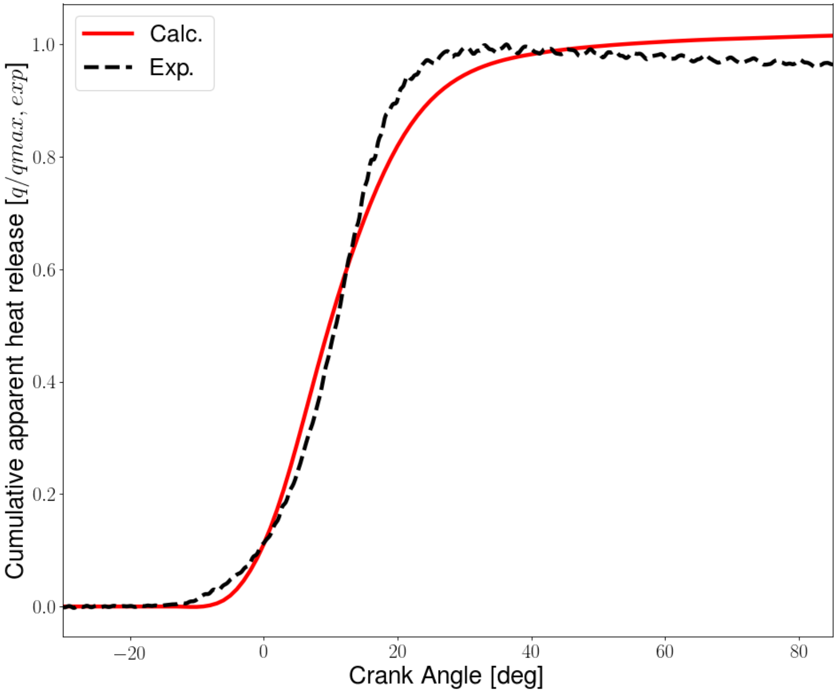
Validation on Heavy-Duty engine



Acceptable agreement between computed and experimental in-cylinder pressure trace.



Auto-ignition under non-premixed conditions: limitations of tabulated kinetics compared to direct integration.

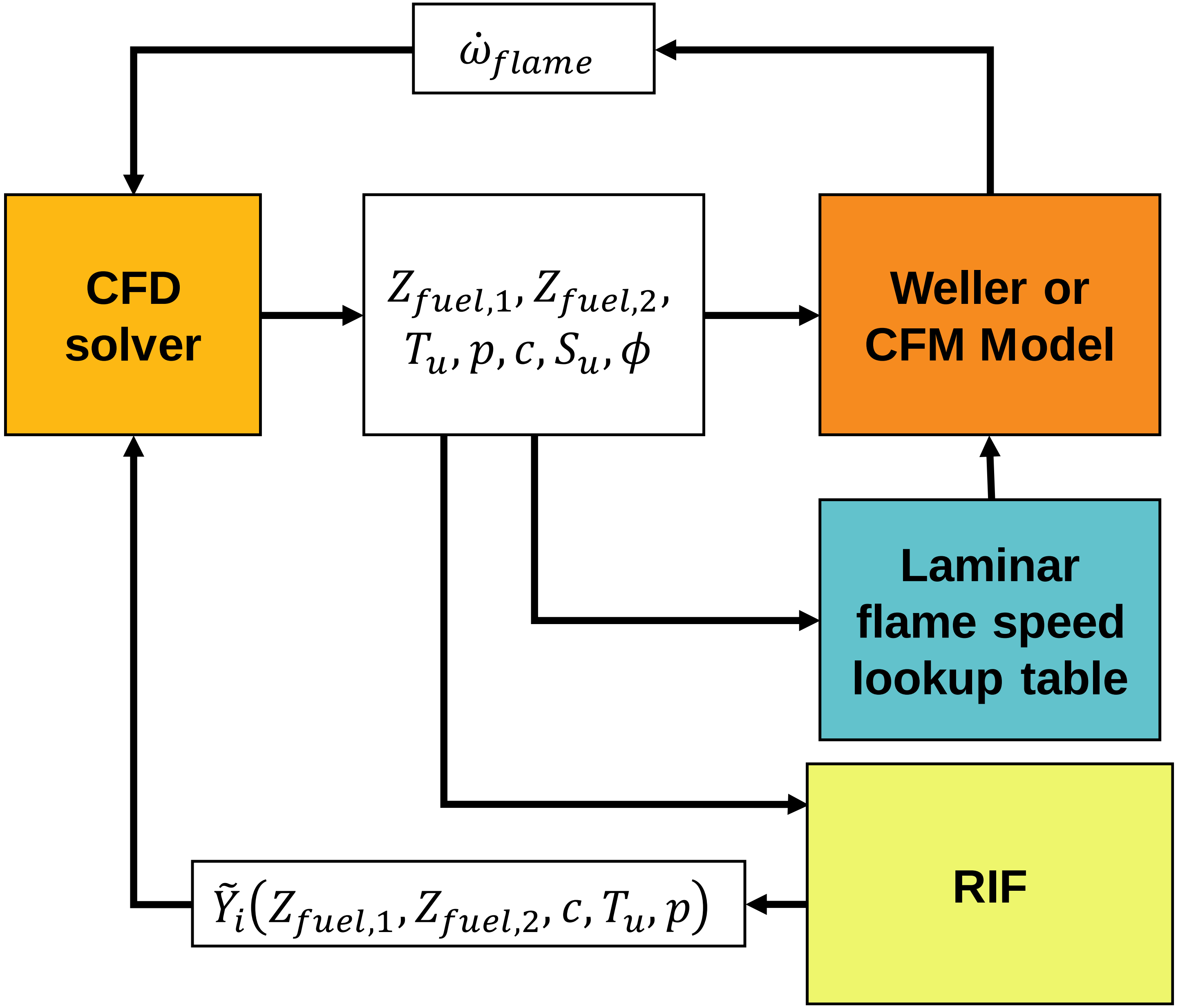


Energy is properly conserved, predicted rate of heat release slower compared to experimental data in the last part of combustion

Dual-fuel combustion

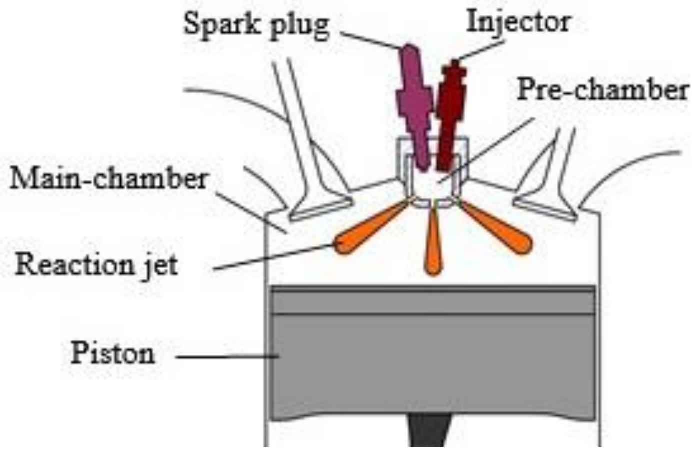
Modeling - future developments

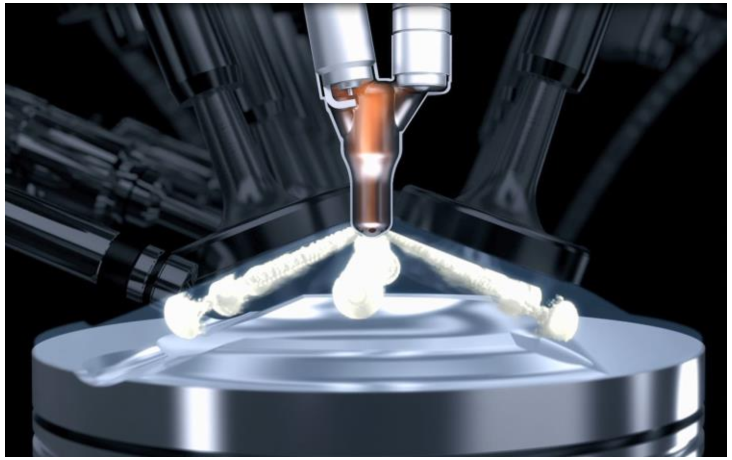
- RIF model to replace homogeneous reactor lookup table:
  - Better description of kinetics and effects of scalar dissipation rate
  - "oxidizer size" ($Z = 0$) with premixed fuel: need to account for chemical reactions taking place in the premixed phase
  - How to switch from auto-ignition to diffusion: progress variable computed in the Z doman and suitable threshold.
- Chemical kinetics: focus on rich conditions with relatively low temperature!



Advanced concepts

Turbulent jet ignition

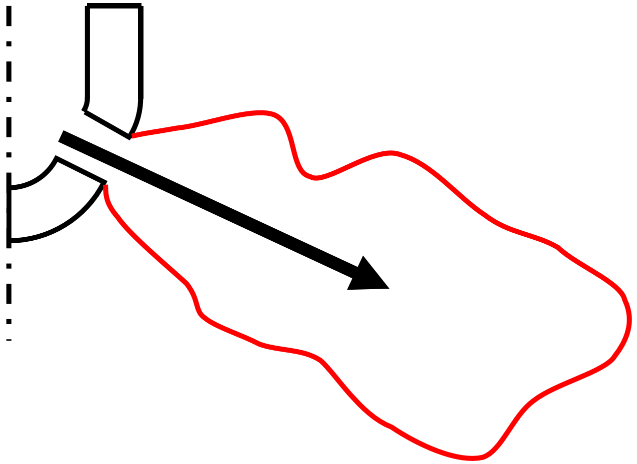




Potentials

- Lean burn combustion ($\lambda > 1.5$) with very reduced emissions
- Advanced combustion modes (spark-assisted combustion)
- Alternative fuels (natural gas, hydrogen)
- Currently employed in very specific engine applications
  - Extension to light-duty engines for efficiency improvement

CFD modeling of pre-chamber, spark-ignition engines: challenges

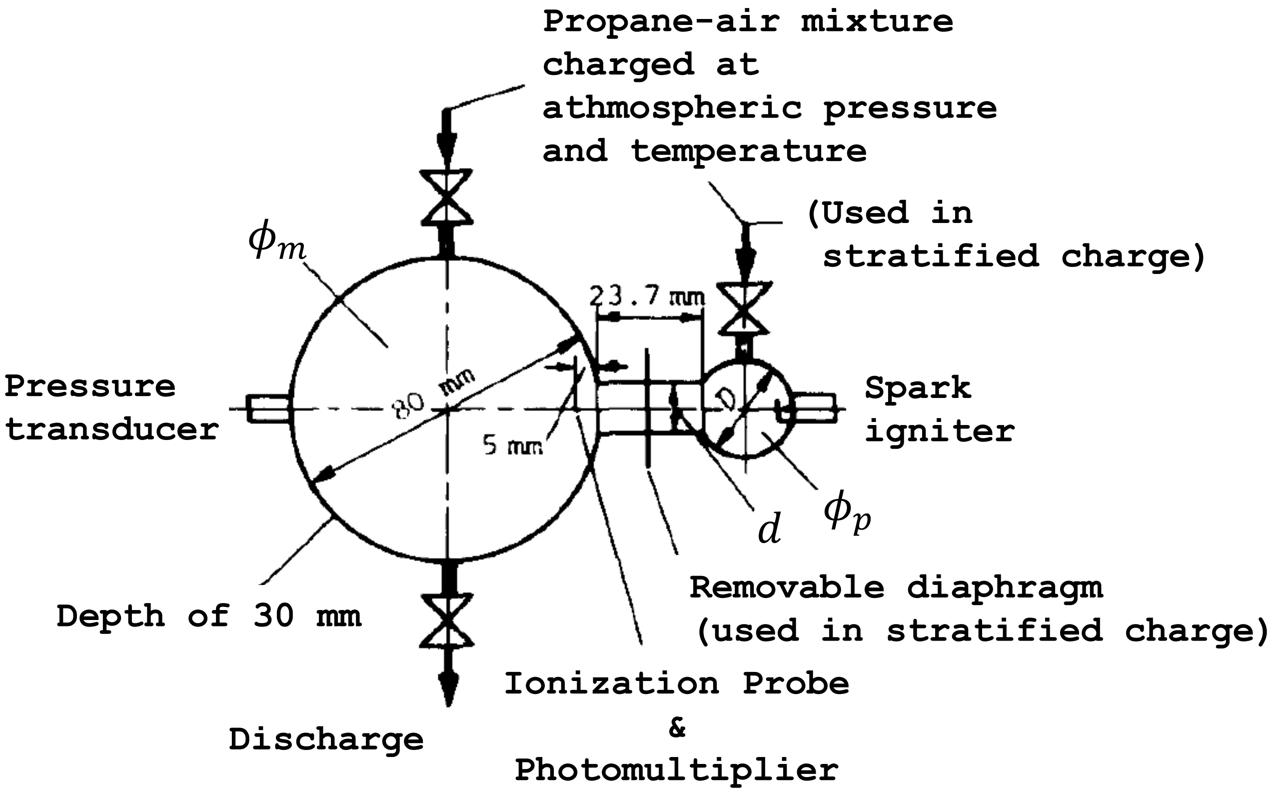


1) Turbulence generation with boundary layer detachment at nozzle inlet
2) Reacting jet penetration
3) Premixed flame propagation in presence of high turbulence generated by the velocity gradients induced by the jet
4) Stratified combustion

Turbulent jet ignition combustion

Experimental database

Yamagouchi et al., *Ignition and Burning process in a divided prechamber bomb*, Comb. Flame 59: 177-185 (1985)



- Fuel: propane
- Chamber initial conditions: $T = 300\ K, p\ =\ 1\ bar$

For a detailed characterization of the combustion process different techniques were employed:

- Schlieren photographs of burning process
- Main chamber pressure evolution
- Ion current histories
- Light emission histories

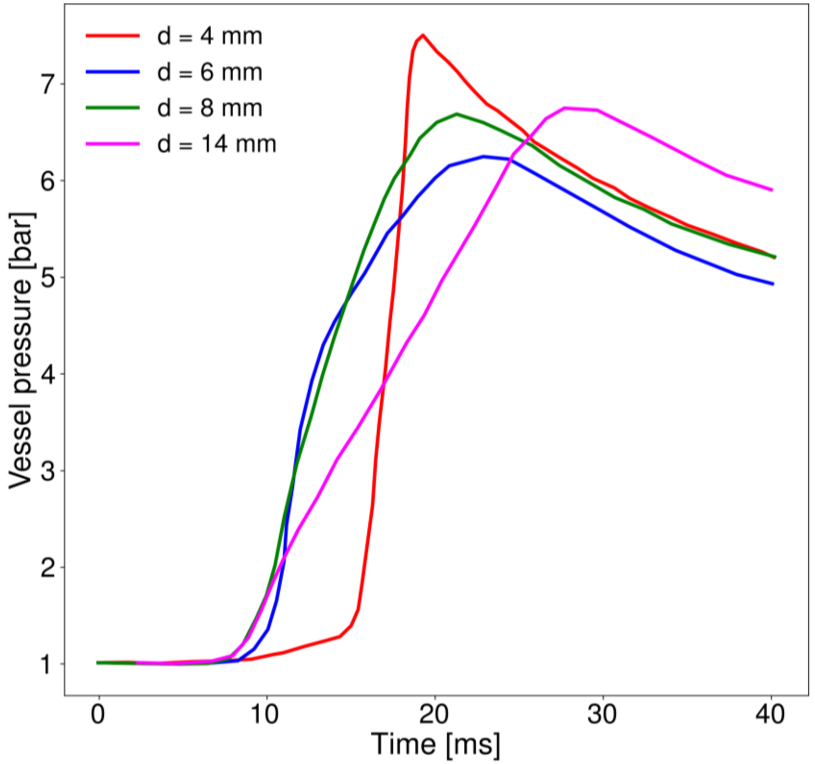
Investigations carried out:

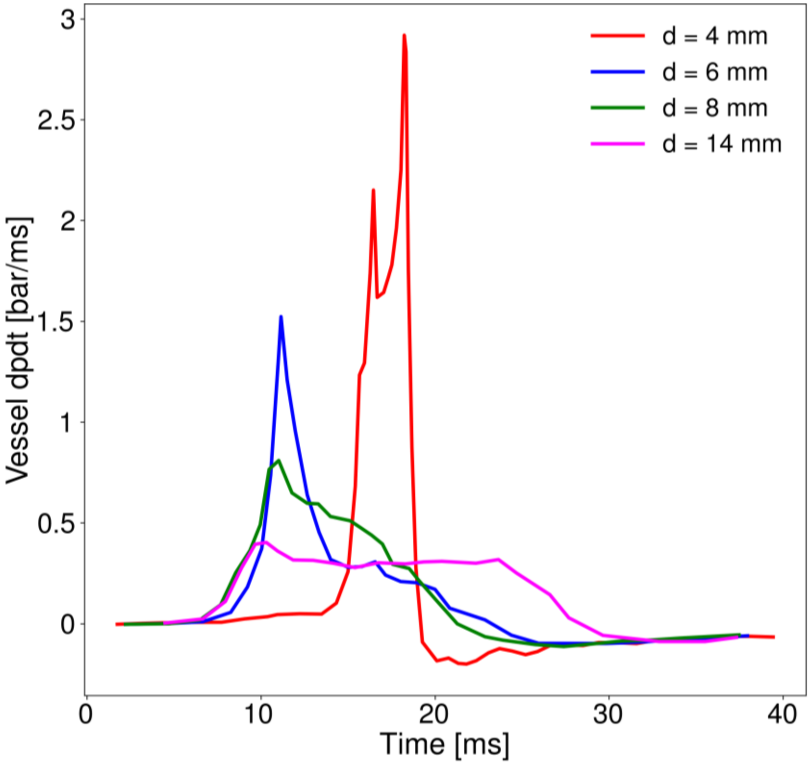
- effect of hole diameter ($4 - 14\ mm$)
- effect of prechamber to main chamber volume ratio ($\frac{V_p}{V_m} = 0.1$ and $\frac{V_p}{V_m} = 0.2$)
- For homogeneous mixture ($\phi_m = \phi_p = 1.1$) and stratified ($\phi_m = 0.6, \phi_p = 1.1$)

Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Operating conditions





Experimental data at V_p/V_m = 0.1

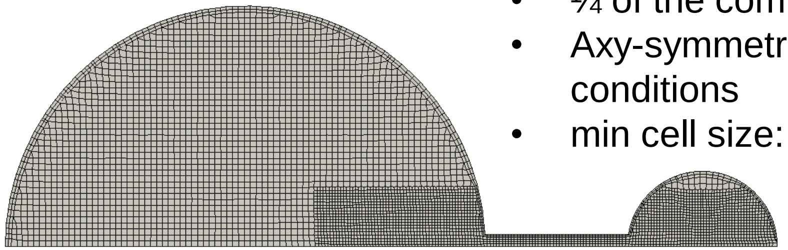
Combustion rate mainly governed by the turbulence generated by the igniting jet:

- $d = 4\,mm$: ignition delay increase almost auto-ignition combustion
- $6\,mm < d < 14\,mm$: increase of combustion duration, reduction of the heat release rate peak.

Simulated operating conditions

	$d = 4\,mm$		$d = 6\,mm$		$d = 8\,mm$		$d = 14\,mm$	
	homog.	strat.	homog.	strat.	homog.	strat.	homog.	strat.
$V_p/V_m = 0.1$	x	x	x	x	x	x	x	x
$V_p/V_m = 0.2$	x		x		x		x	

Computational mesh



- ¼ of the combustion chamber
- Axy-symmetric boundary conditions
- min cell size: 0.5 mm

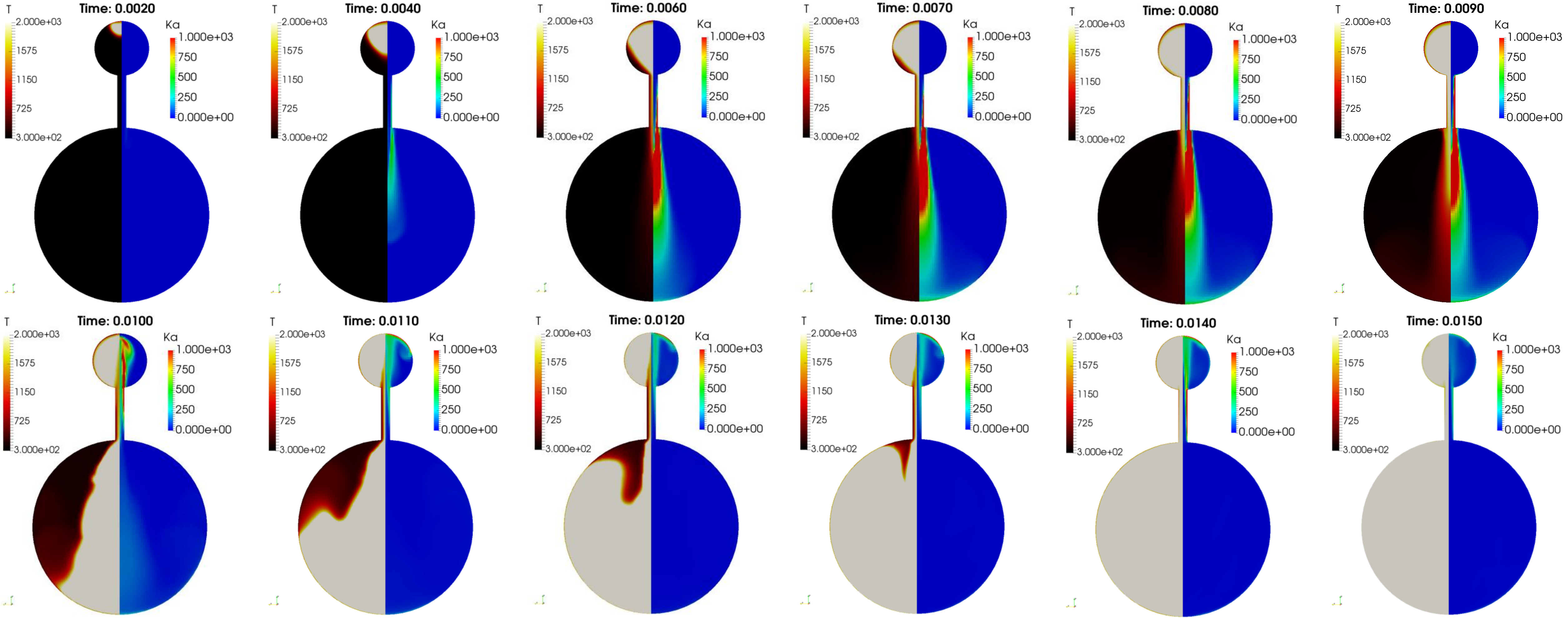
Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Analysis of combustion regimes

Simulation for $d = 0.4\,mm$, $V_p/V_c = 0.1$, $\phi = 1.1$ (homogeneous)

Evolution of temperature and Karlovitz number fields



Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Analysis of combustion regimes

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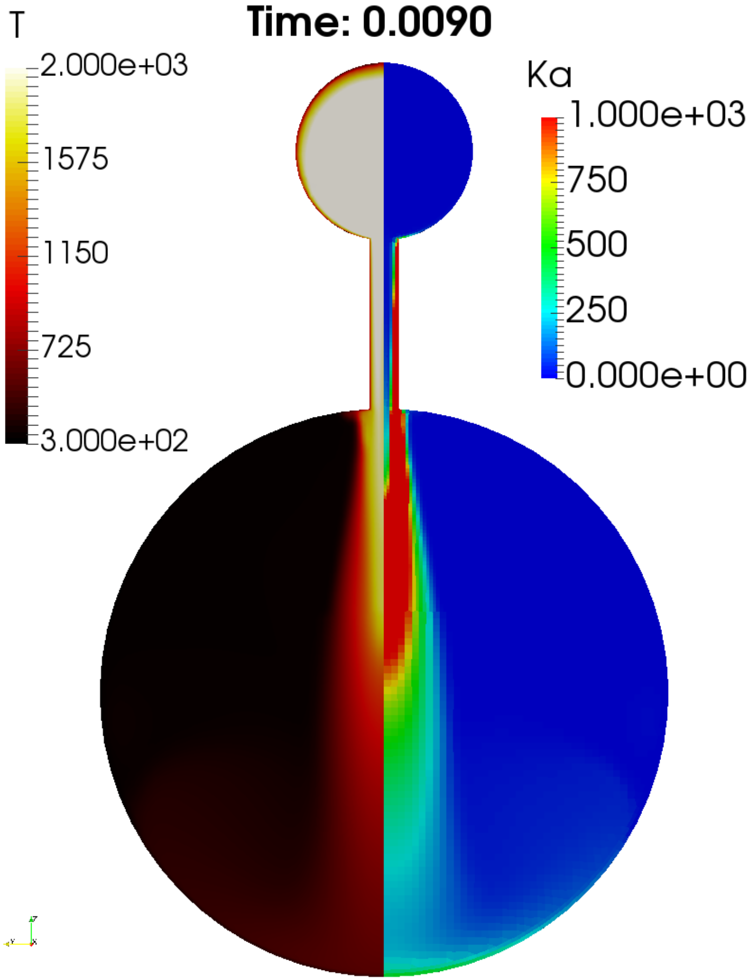
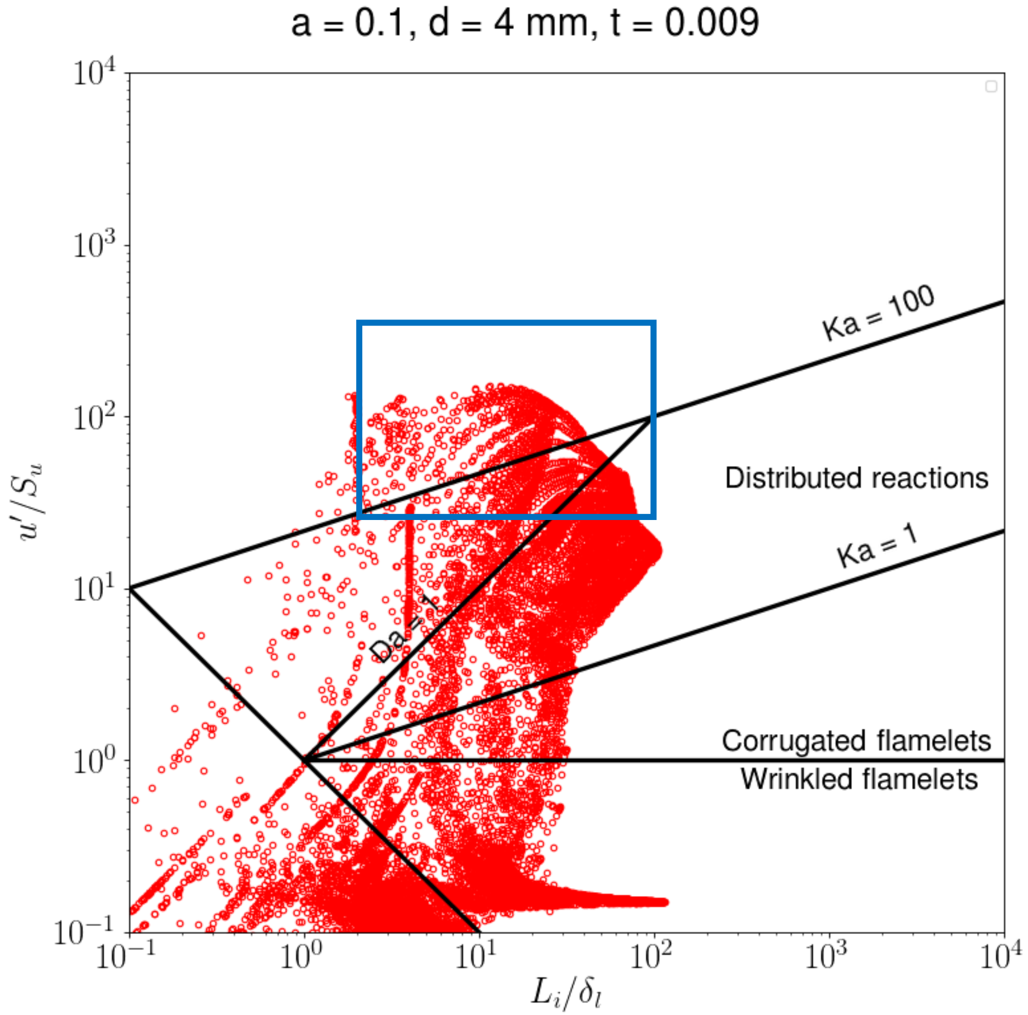




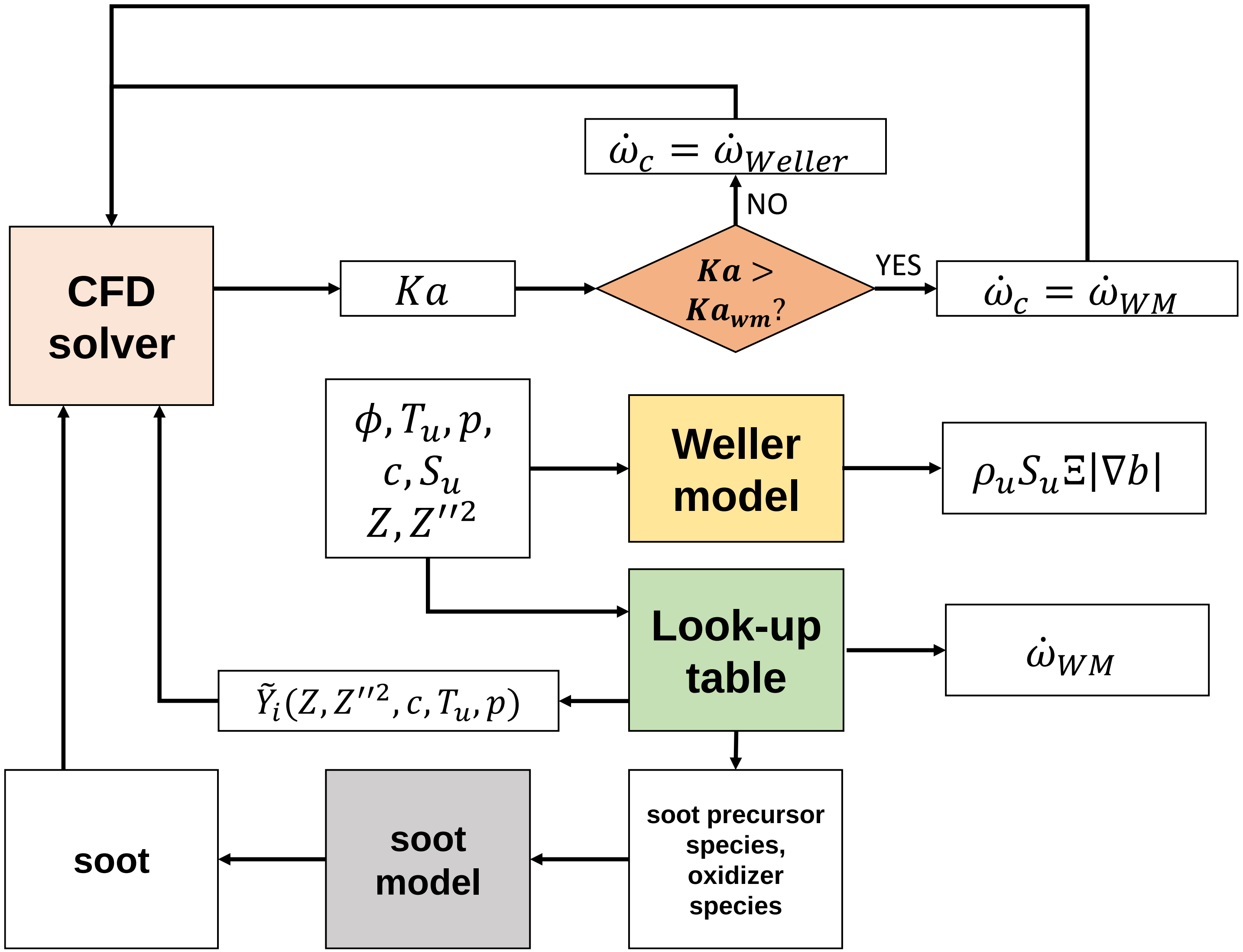
Karlovitz number goes well above 1000 when the hot jet enters the main chamber.

Expected combustion regimes are, in simulation, strongly affected by:

- predicted levels of turbulence (turbulence model)
- estimated value of the laminar flame speed (from correlation or estimated by detailed mechanisms).

Turbulent jet ignition combustion

Combustion model concept



CFD solver

Ka

$Ka > Ka_{wm}$?

NO

$\dot{\omega}_c = \dot{\omega}_{Weller}$

YES

$\dot{\omega}_c = \dot{\omega}_{WM}$

$\phi, T_u, p,$
c, S_u
Z, Z''^2

Weller model

$\rho_u S_u \Xi |\nabla b|$

Look-up table

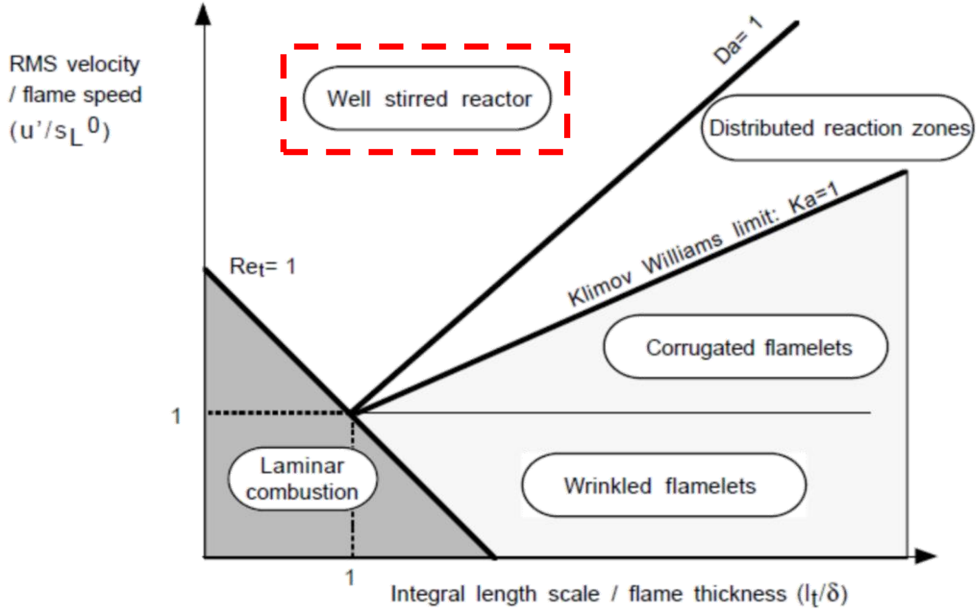
$\dot{\omega}_{WM}$

$\tilde{Y}_i(Z, Z''^2, c, T_u, p)$

soot precursor species, oxidizer species

soot model

soot



Poinsot, Veynante, *Theoretical and Numerical Combustion*, Edwards, 2005

Handling transition from distributed to well-stirred reactor model:

- if $Ka > Ka_{wm}$
  → Reaction rates from lookup table (well mixed or presumed PDF)
- else
  → Weller model

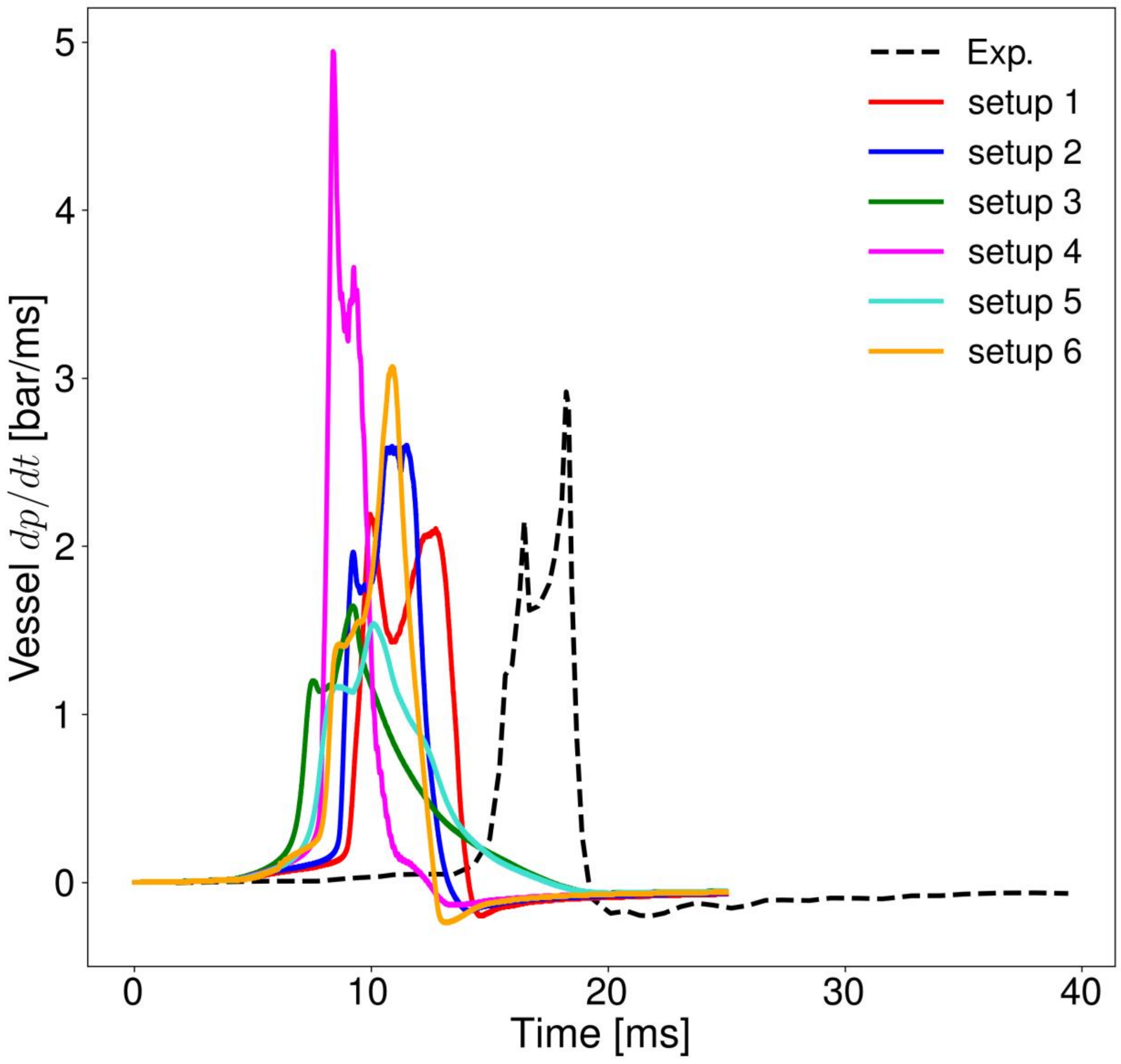
Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $d = 0.4\,mm$, $V_p/V_c = 0.1$, $\phi = 1.1$ (homogeneous)

	Turbulence model	**S_t/S_l correlation**	Ka_{wm}	**Ξ model**
setup 1	$k-\omega$ SST	Peters	1000	Two-equation
setup 2	$k-\omega$ SST	Peters	1000	**Algebraic**
setup 3	$k-\omega$ SST	Peters	∞	**Algebraic**
setup 4	$k-\omega$ SST	**Gulder**	∞	Two-equation
setup 5	$k-\omega$ SST	Peters	∞	Two-equation
setup 6	$\boldsymbol{k-\varepsilon}$ $(\mathbf{C_1 = 1.55})$	Peters	1000	Two-equation

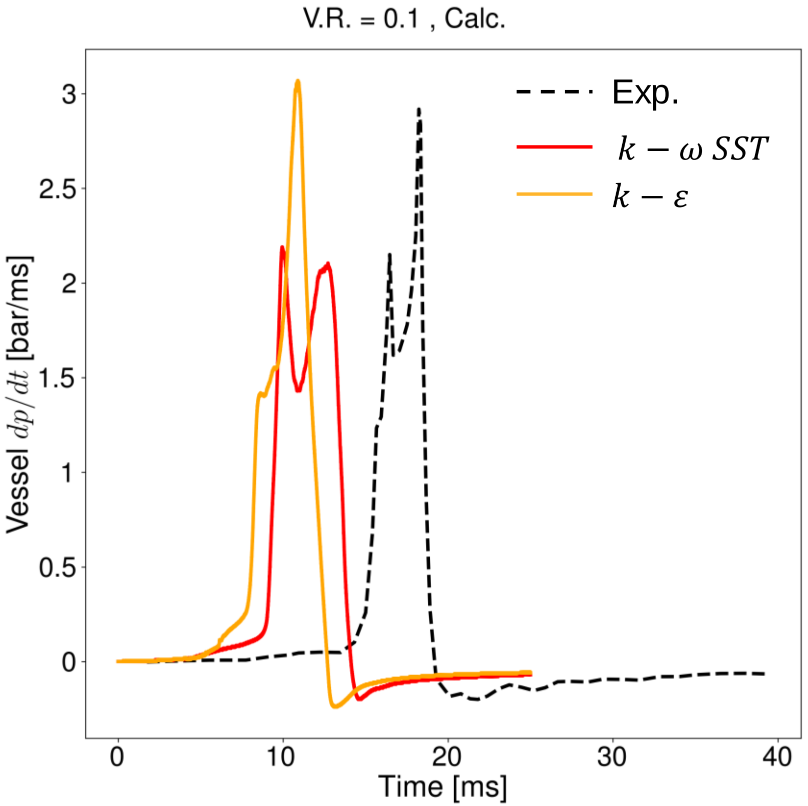
- Different results from the adopted setup, despite the reacting jet penetration is similar.
- Underestimated ignition delay (very low initial chamber temperature and pressure).
- Peters correlation works better compared to the Gulder's one.



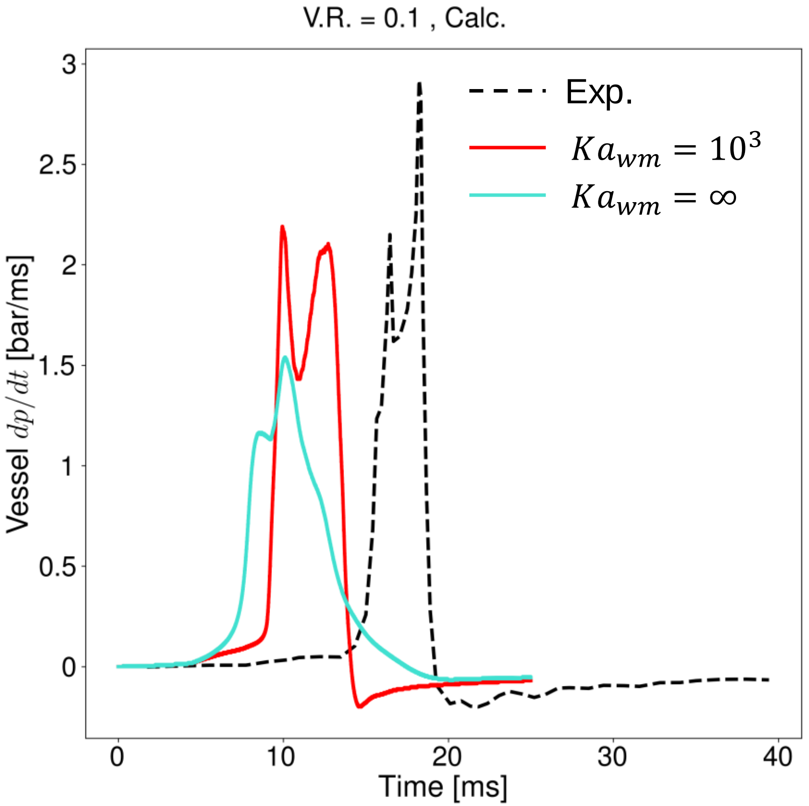
Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

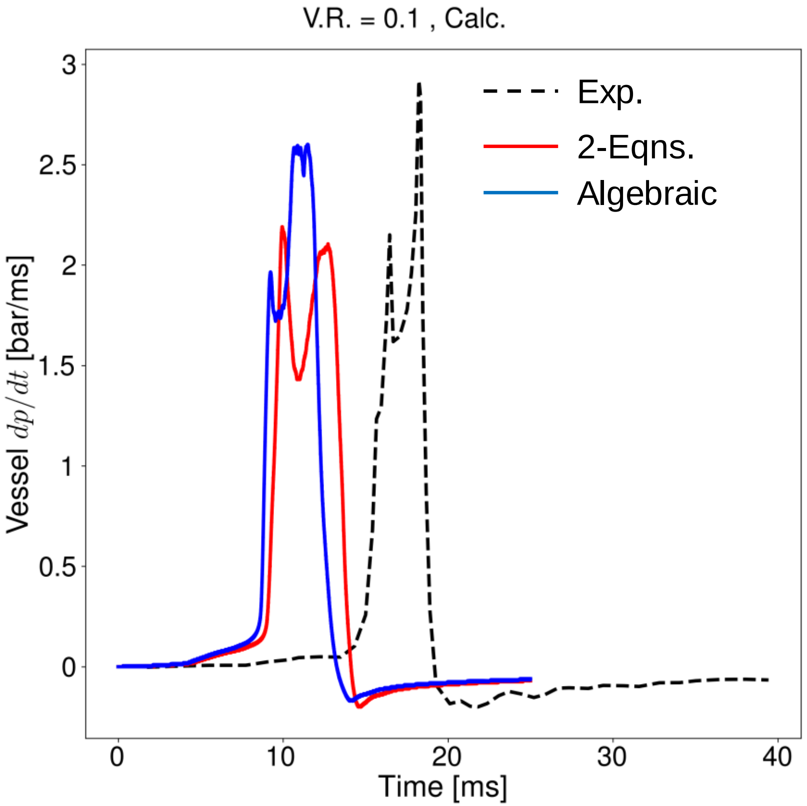
Combustion model validation: $d = 0.4\,mm$, $V_p/V_c = 0.1$, $\phi = 1.1$ (homogeneous)



$k-\omega\ SST$ qualitatively better describes the experimental heat release rate profile compared to $k-\varepsilon$ model. Ignition delay also increases with $k-\omega\ SST$



Accounting for well-stirred reactor combustion regime produces a better estimation of the ignition delay and description of the heat release rate profile.

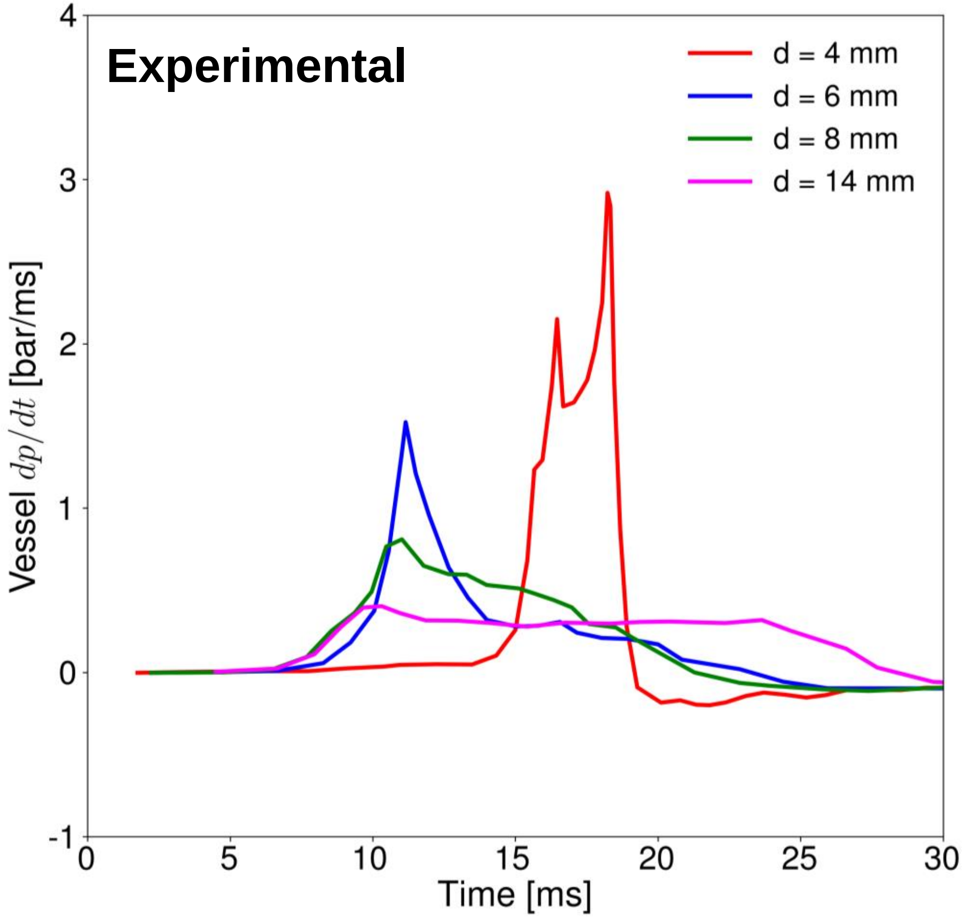


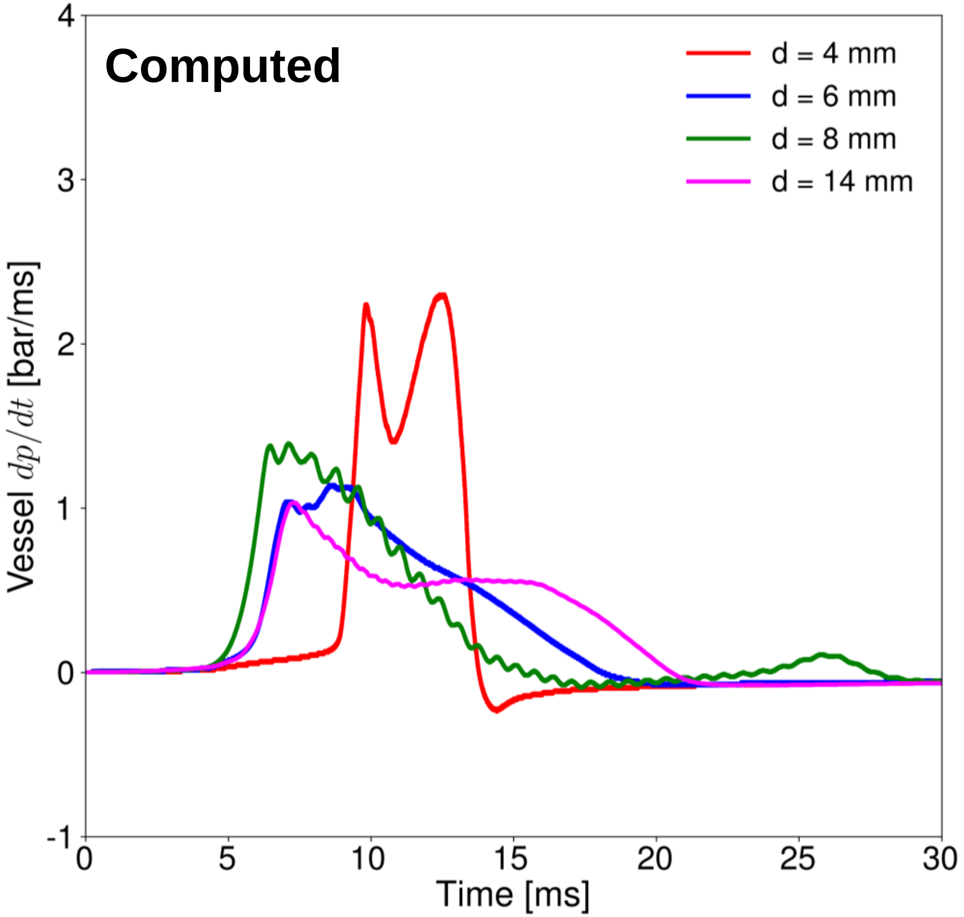
Two equation model better than the algebraic formulation both in terms of ignition delay prediction and heat release rate profile.

Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $V_p/V_c = 0.1$, $\phi = 1.1$ (homogeneous)





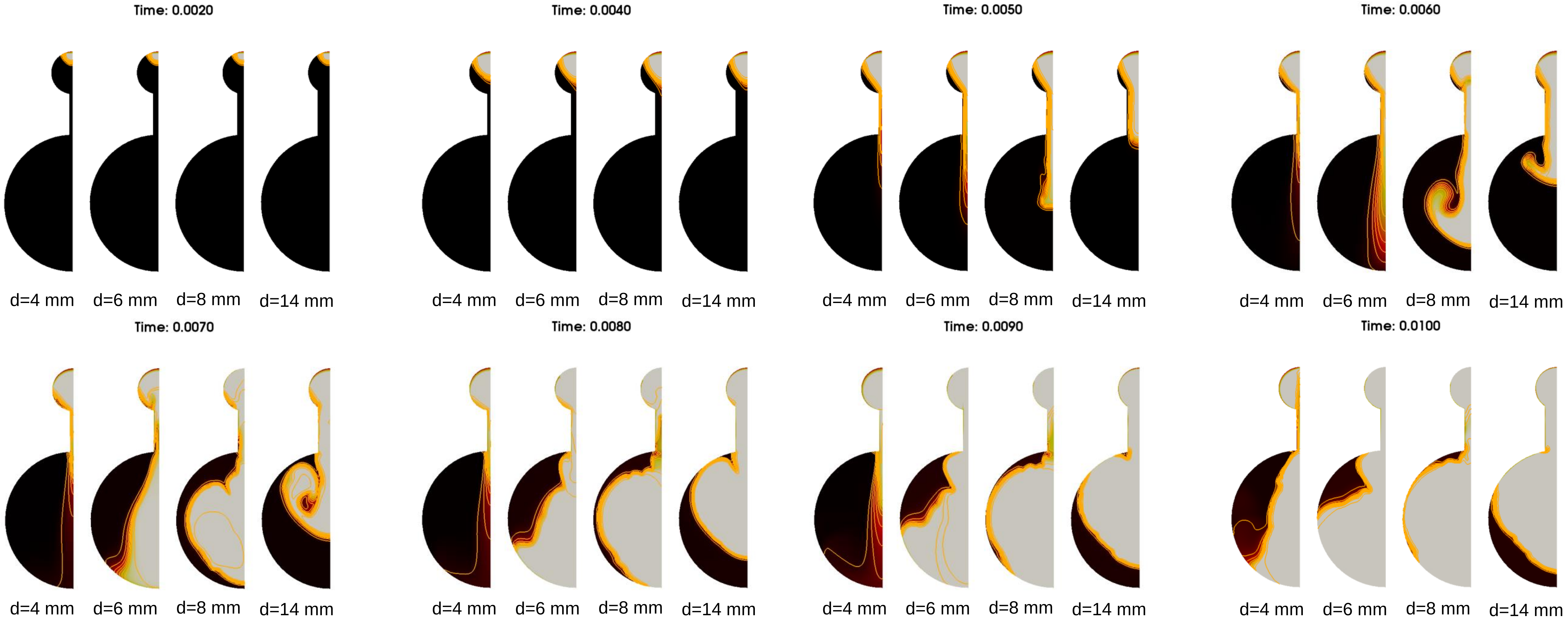
+ Increased ignition delay for d = 4.0 mm condition
+ Similar ignition delays for d = 6, 8, 14 mm

+ Increased combustion duration for d = 14 mm
- Variation from 6 to 8 mm not captured by the model

Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $V_p/V_c = 0.1$, $\phi = 1.1$ (homogeneous)

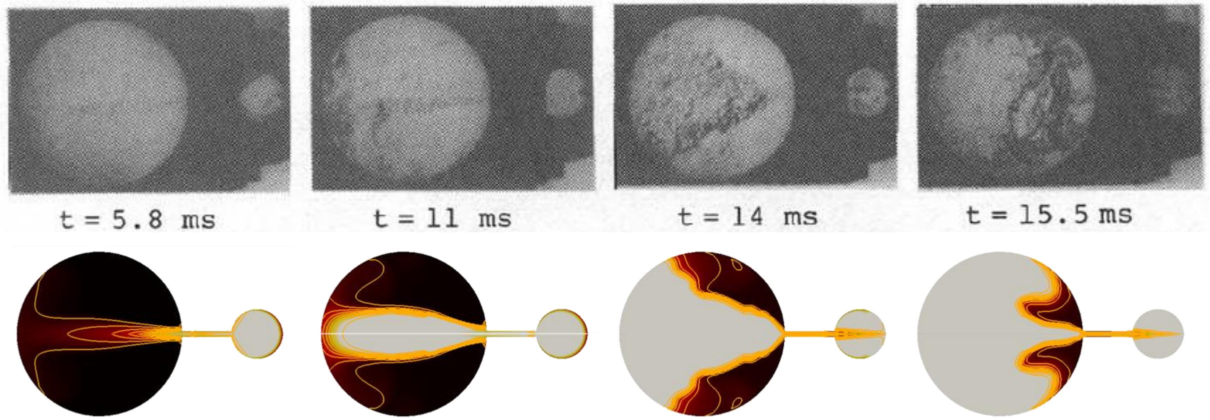


Turbulent jet ignition combustion

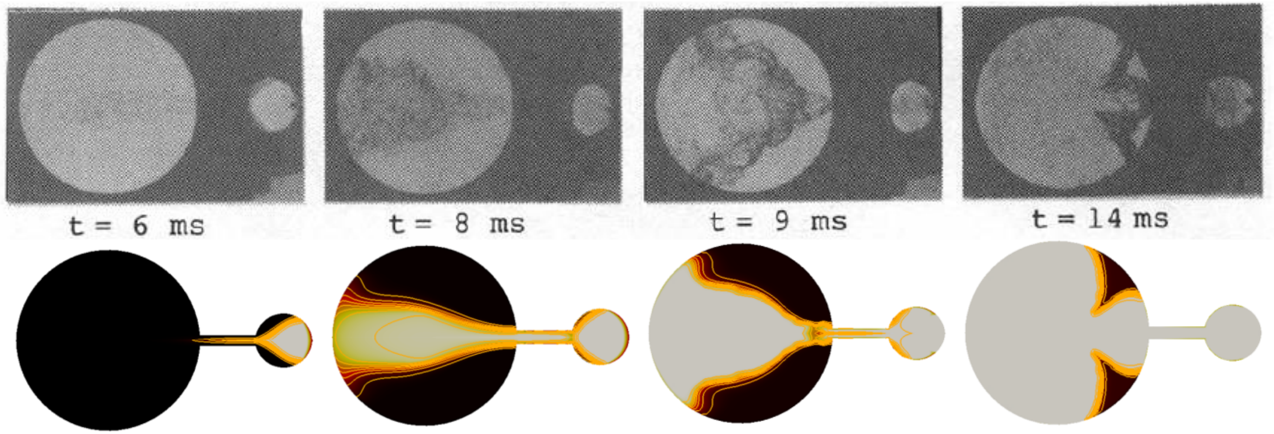
Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $V_p/V_c\ =\ 0.1,\ \phi = 1.1$ (homogeneous)

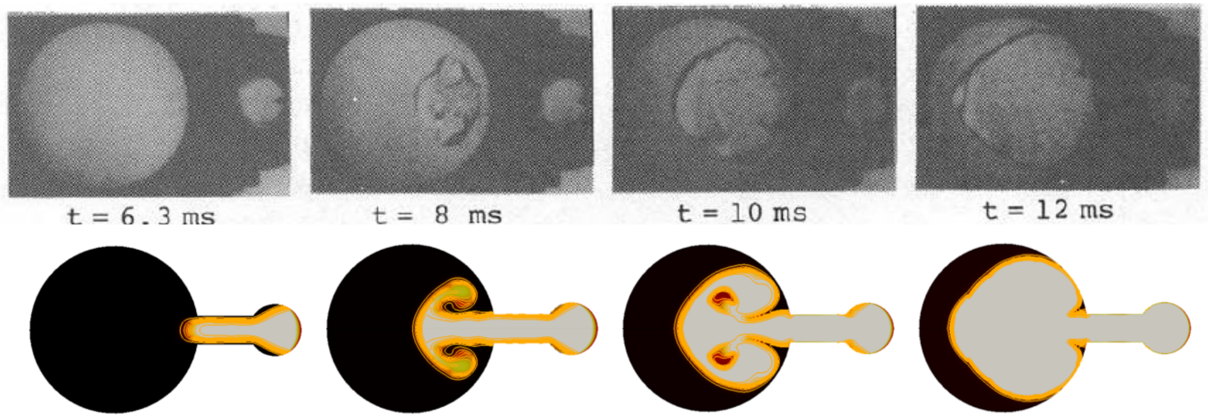
d = 4 mm: Ignition sequence



d = 6 mm: Ignition sequence



d = 14 mm: Ignition sequence

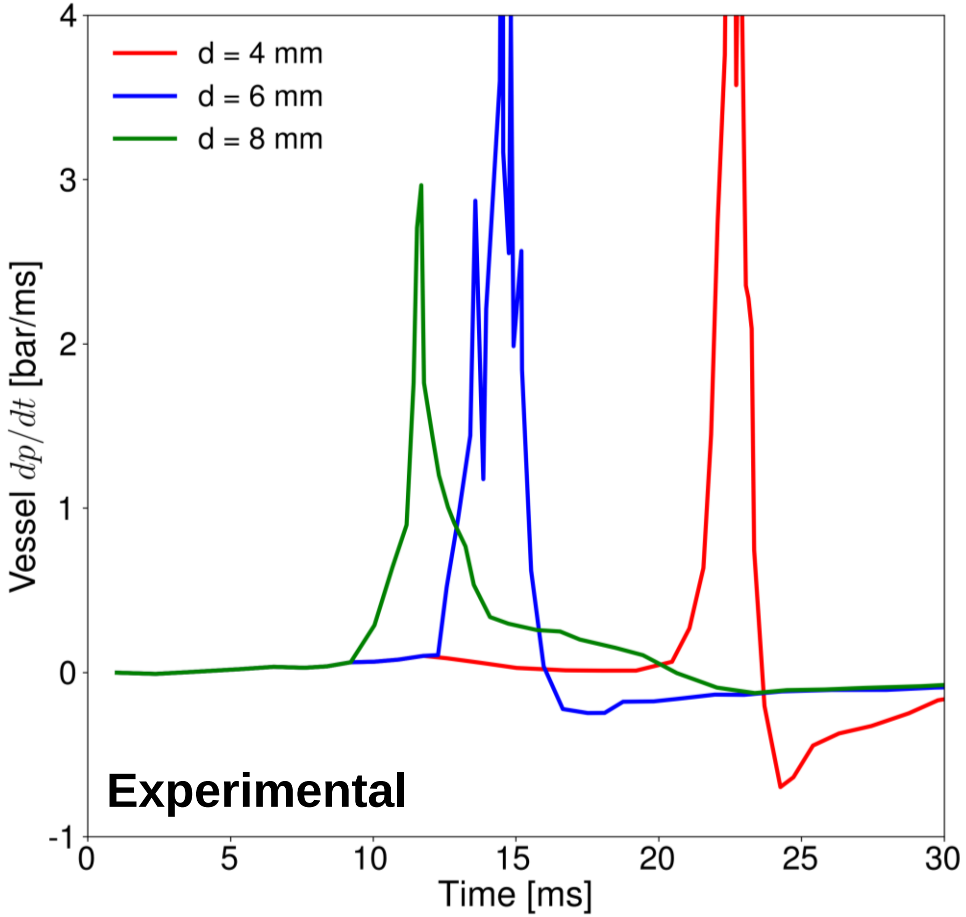


Change in flame morphology correctly described by the model

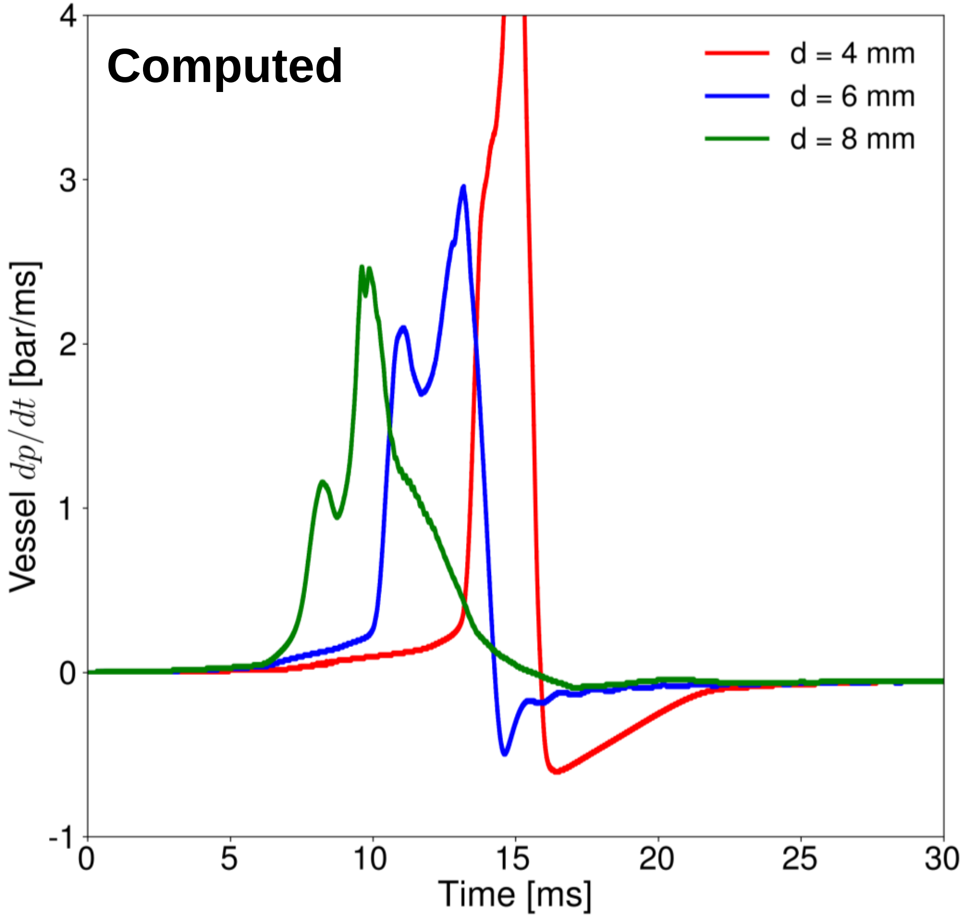
Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $V_p/V_c = 0.2$, $\phi = 1.1$ (homogeneous)



- \+ Effect of increased prechamber volume is similar to those of reducing the nozzle diameter.

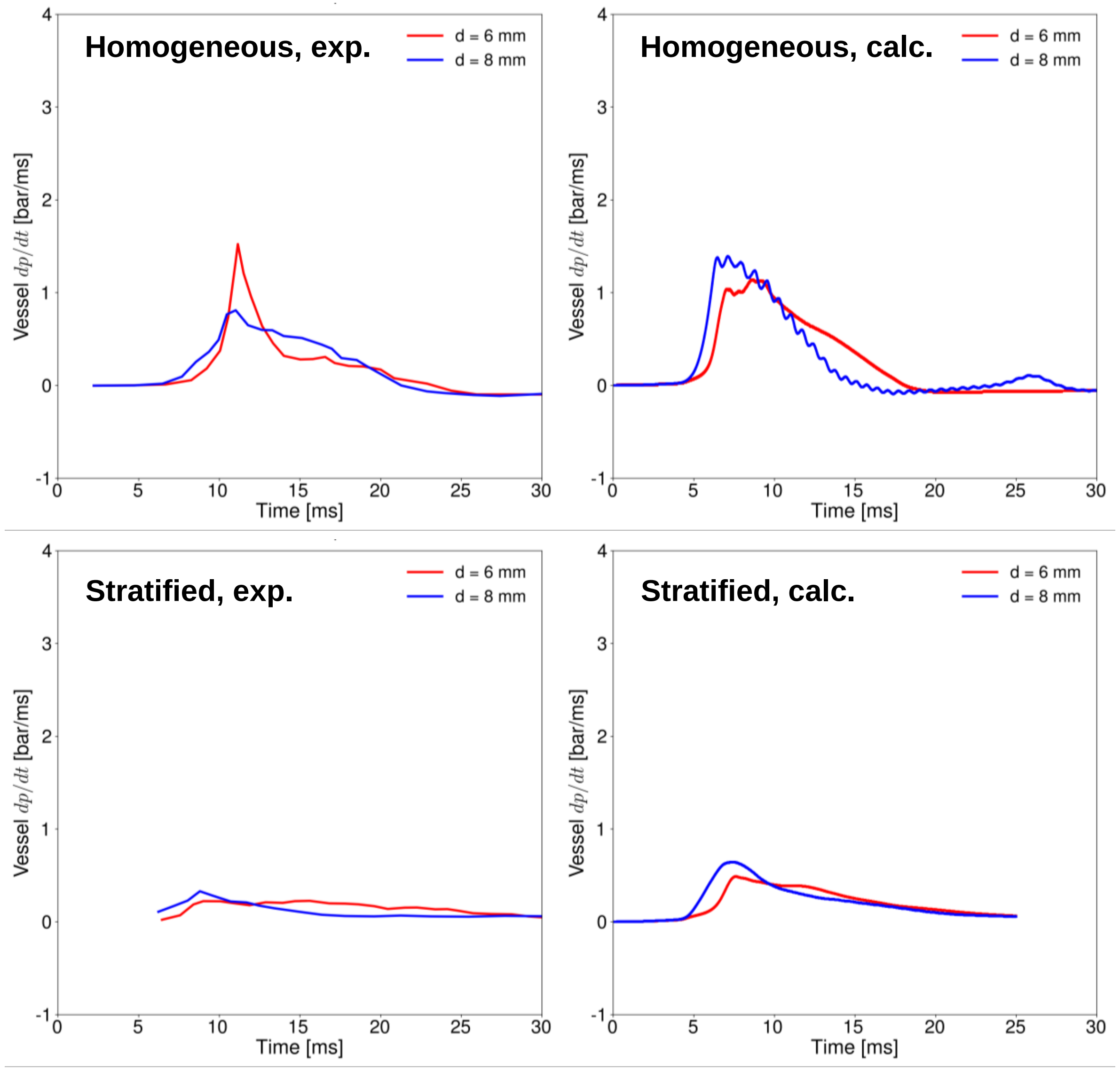


- \+ Increase of nozzle diameter reduces the ignition delay.

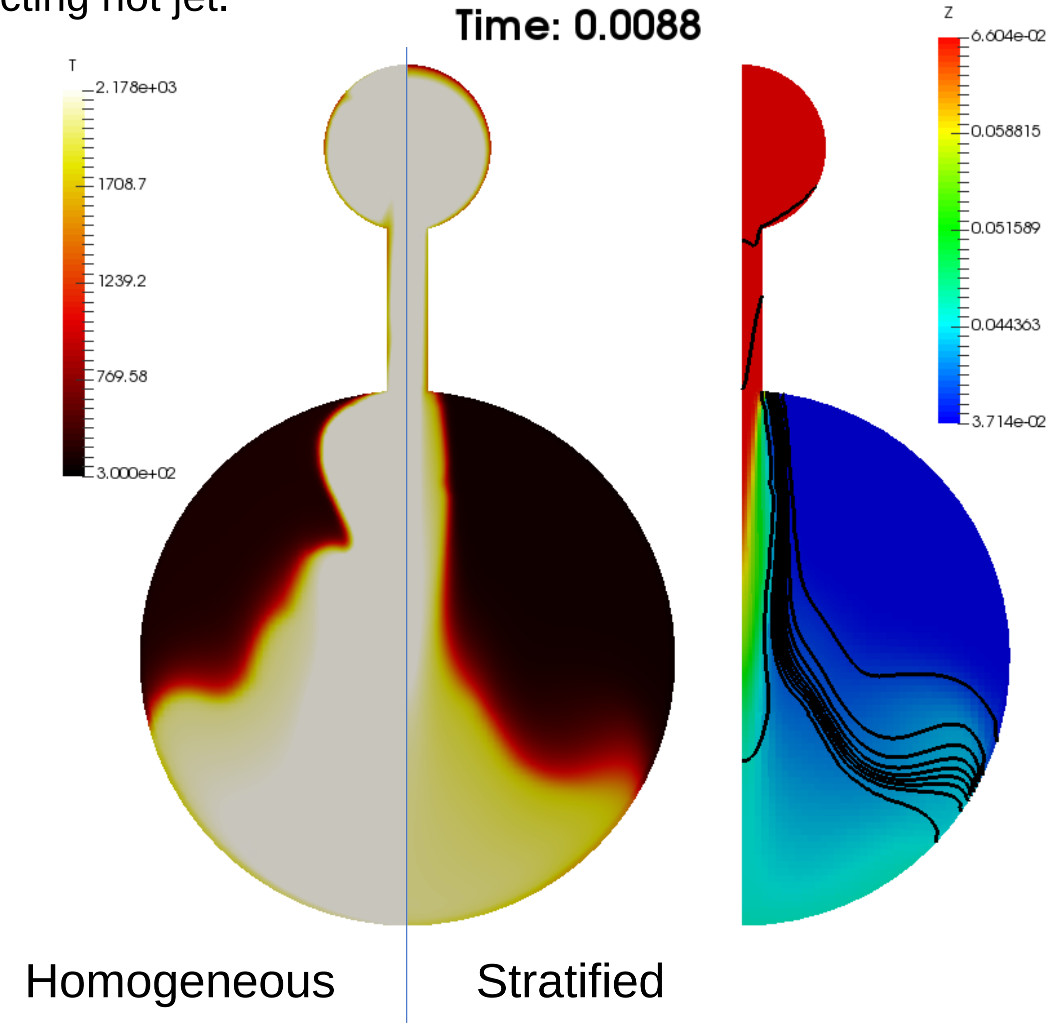
Turbulent jet ignition combustion

Exp. data in: Yamacouchi et al, Comb. Flame, 1985

Combustion model validation: $V_p/V_c = 0.1$, $\phi_p = 1.1, \phi_m = 0.6$ (stratified)



- Simulations correctly estimate ignition of the lean mixture by the reacting hot jet.



Conclusions

Modeling of premixed combustion in conventional and innovative engines

Weller combustion model

- Predictive capability for both Algebraic and 2-Equation approaches.
- Attention to laminar to turbulent flame transition:
    - Tabulation of Markstein Lenghts
    - Laminar flame speed estimation at high pressure conditions

Conventional SI combustion

- Four different configurations successfully tested
- Combustion model matters but...
    - turbulence, flow and mixture distribution must be correctly estimated.
- A lot of work to be done on emissions:
    - Soot from pool fires (ECN), NOx, HC.

Advanced combustion concepts

- Dual fuel combustion model performs rather well, but:
    - Auto-ignition – RIF?
    - Smooth transition to premixed combustion?
- Turbulent-jet ignition:
    - Need to model different combustion regimes
    - Turbulence model and wrinkle factor correlation matters.

Thanks for your attention!

GROUP
POLITECNICO DI MILANO