libEngine: C++ object-oriented platform for in-cylinder flow and combustion modeling

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`http://www.engines.polimi.it`

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Topics

- The OpenFOAM® technology
- The libEngine project: an overview
    - 1D-3D coupling
    - Diesel exhaust after-treatment modeling
    - In-cylinder flow and combustion models
- Diesel combustion modeling in libEngine
    - Mesh management
    - Spray modeling
    - Combustion

The OpenFOAM technology

- OpenFOAM: open-source, object oriented CFD code developed by OpenCFD.

- Ideal tool to perform applied and fundamental studies:
  - Open-source
  - Object-oriented
  - Wide range of pre-implemented capabilities (discretization, mesh management, numerical and physical models)

The OpenFOAM technology

Open-source

- Research work performed in a collaborative environment:
  - ➢ Exchange of sub-routine and applications among different research groups.
  - ➢ Possibility to implement different models (spray, combustion,…) on the same platform and easily compare them.

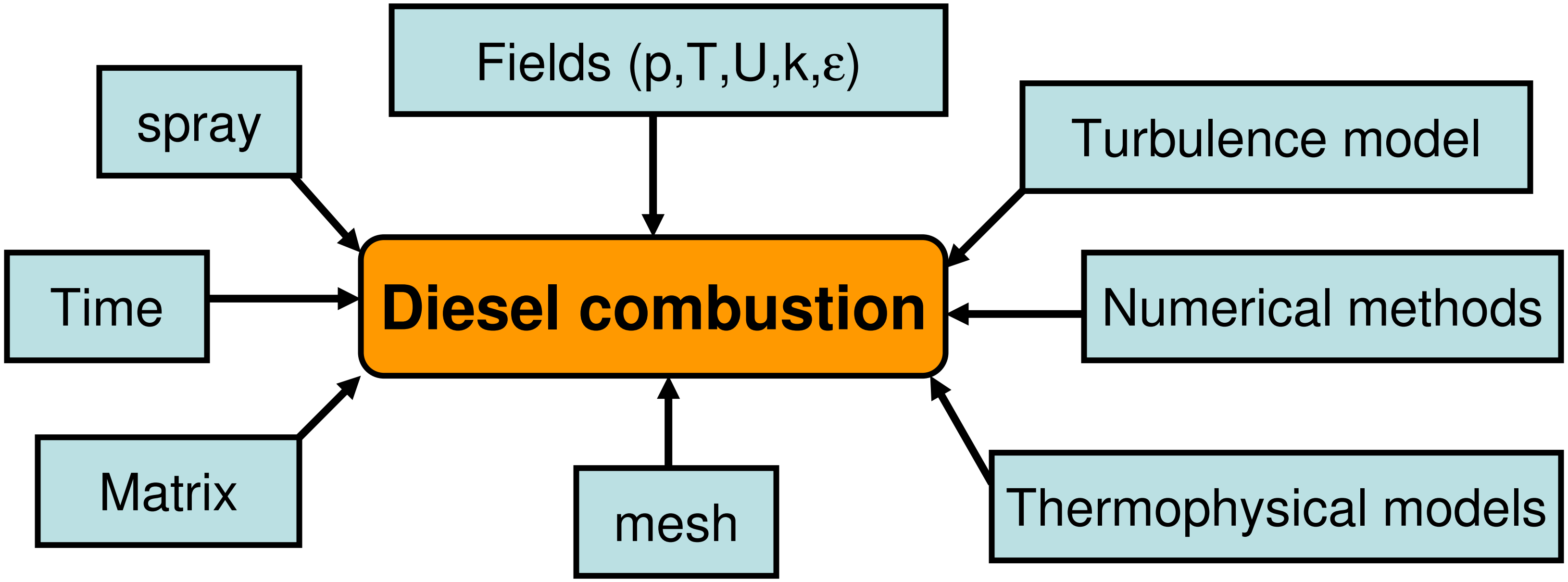
Object-oriented CFD (C++ language)

- Avoid global data corruption (private, public and protected data).
- The code is composed by small manageable units (Classes)
- **Class**: user defined type representing one part of the problem I have to solve (mesh, matrix, field, ..).
- **Library**: definition and implementation of related classes and functions (finite volume library, turbulence model library, mesh tools library…).
- **Application**: collection of object of different classes interacting each others and “doing various things”.

The OpenFOAM technology

Object-oriented CFD (C++ language)

Object-oriented modeling of diesel combustion:
Introduce new data types (*classes*) appropriate for the problem



Fields (p,T,U,k,ε)

spray

Turbulence model

Time

Diesel combustion

Numerical methods

Matrix

mesh

Thermophysical models

The OpenFOAM technology

Object-oriented CFD (C++ language)

Field-Operation And Manipulation (FOAM): representing the PDE systems in their natural language:

Scalar transport equation: $\boxed{\frac{\partial \rho Y}{dt} + \nabla \cdot \left(\rho \mathbf{U} Y\right) - \nabla \cdot \left(\upsilon \nabla Y\right) = \rho \dot{Y}}$

- Implementation in OpenFOAM

```
solve
(
        fvm:ddt(rho, Y)
-       fvm:div(phi, Y)
-       fvm::laplacian(nu, Y)
==
        rho*Ydot
)
```

The OpenFOAM technology

Pre-implemented capabilities

OpenFOAM library:

- Finite-volume discretization with polyhedral cell support
- Finite-element mesh motion + topological changes
- Lagrangian particle tracking algorithm
- Thermophysical (liquid and gases) models
- Detailed chemistry…

OpenFOAM applications/solvers:

- **Compressible flow solvers**: RANS, LES, pressure-density based, density based, steady, unsteady
- **Combustion**: premixed or non-premixed combustion models
- **heatTransfer**: solvers for buoyancy-driven or Bousinnesq flows
- **Incompressible flows**: (steady, unsteady, viscid, inviscid, RANS, LES, …)

OpenFOAM-related CFD projects

OpenFOAM

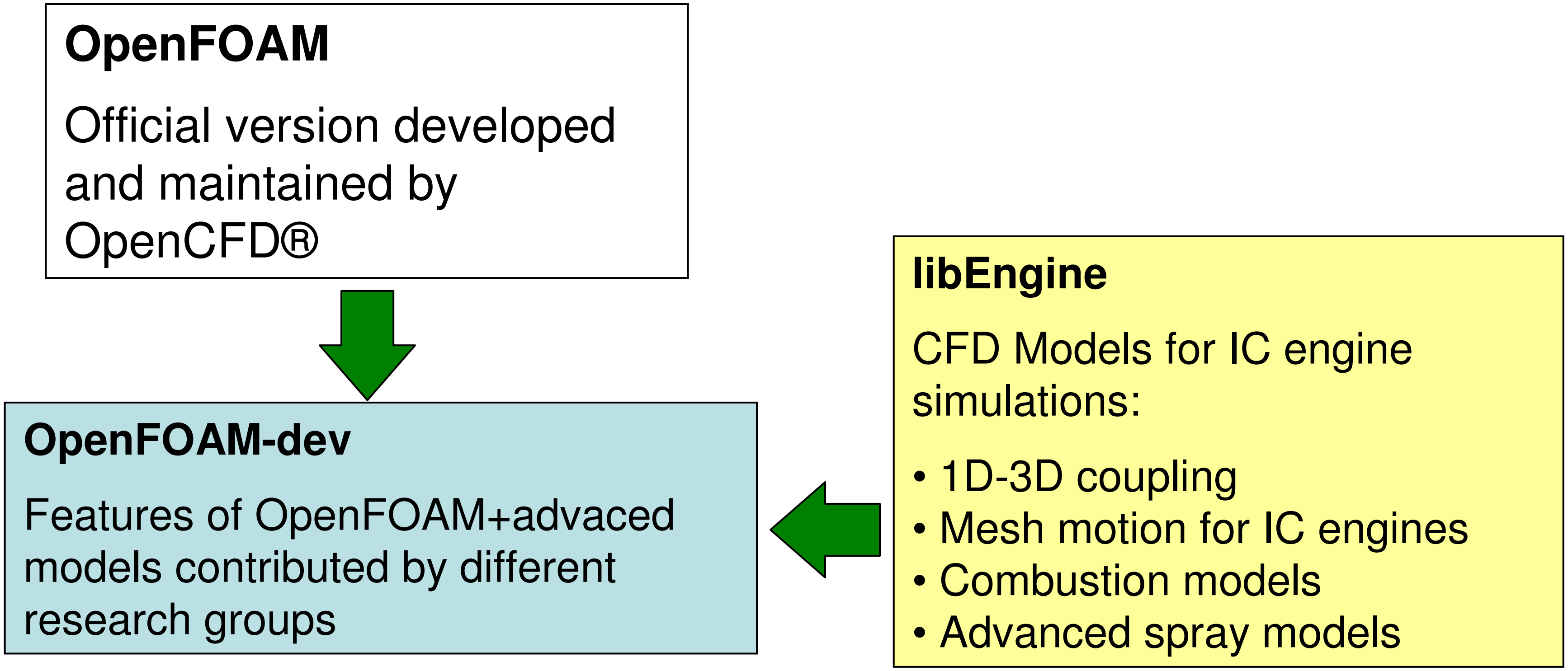
Official version developed and maintained by OpenCFD®

OpenFOAM-dev

- All the basic features of the official OpenFOAM versions
- Advanced applications/libraries contributed by different groups:
  - Wikki Ltd. (Prof. H. Jasak)
  - Chalmers University of Technology (Prof. H. Nilsson)
  - Politecnico di Milano
  - University of Zagreb (Dr. Z. Tukovic)
  - Penn-State University (Prof. E. Patterson)
  - ICE (Dr. B. Gshaider)
  - …

libEngine

- Based on the OpenFOAM technology
- Specific libraries, applications and utilities developed for IC engine simulations.



OpenFOAM

Official version developed and maintained by OpenCFD®

OpenFOAM-dev

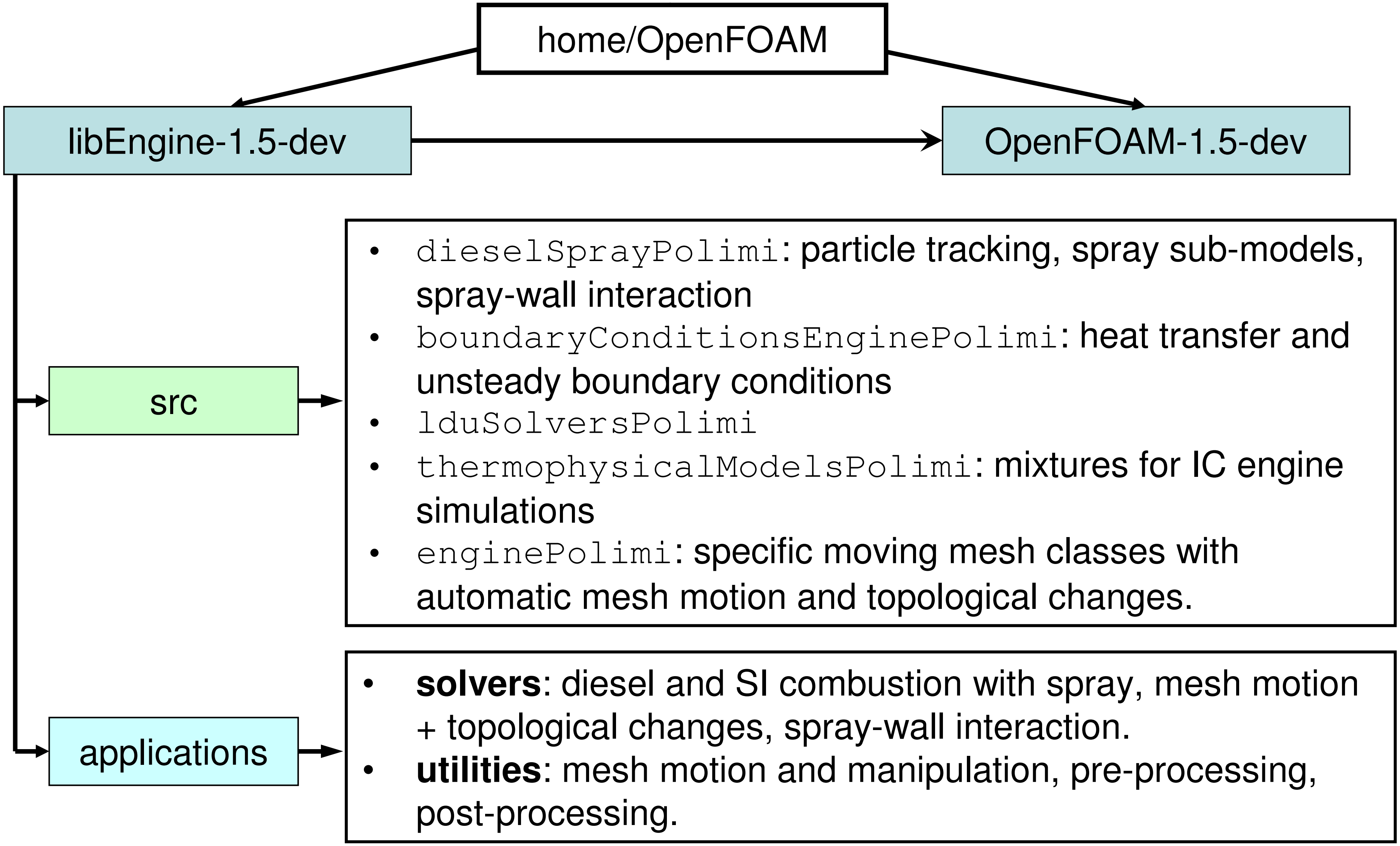
Features of OpenFOAM+advaced models contributed by different research groups

libEngine

CFD Models for IC engine simulations:

- 1D-3D coupling
- Mesh motion for IC engines
- Combustion models
- Advanced spray models

libEngine



home/OpenFOAM

libEngine-1.5-dev

OpenFOAM-1.5-dev

src

- `dieselSprayPolimi`: particle tracking, spray sub-models, spray-wall interaction
- `boundaryConditionsEnginePolimi`: heat transfer and unsteady boundary conditions
- `lduSolversPolimi`
- `thermophysicalModelsPolimi`: mixtures for IC engine simulations
- `enginePolimi`: specific moving mesh classes with automatic mesh motion and topological changes.

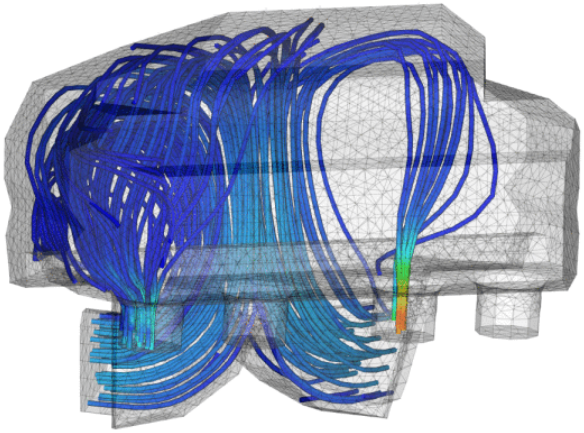
applications

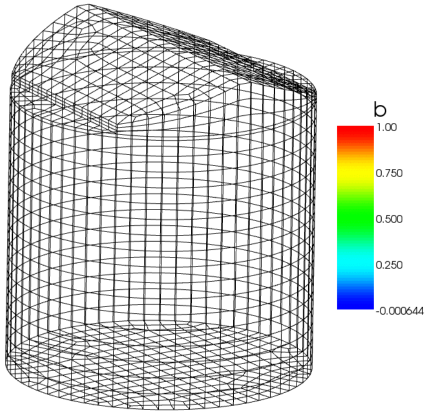
- **solvers**: diesel and SI combustion with spray, mesh motion + topological changes, spray-wall interaction.
- **utilities**: mesh motion and manipulation, pre-processing, post-processing.

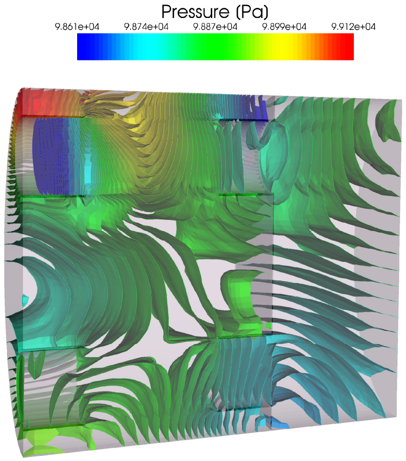
libEngine

1D-3D coupling

- Fully integrated 1D-3D simulation of the whole engine system.
  - Intake and exhaust systems
  - Closed-valve in-cylinder flow modeling
- Coupling strategy based on the solution of the Riemann problem at the 1D-3D interface.
- OpenFOAM successfully coupled with GASDYN (2006) and GTPower (2008).







libEngine

Diesel exhaust-after treatment modeling

- Full scale DPF modeling: optimizing the DPF geometry accounting for flow non-uniformities (Fig. 1).
- Automatic-mesh generation of DPF geometries accounting for the different components (plug-ends, filter channels and chessboard arrangement) (Fig. 2).
- Momentum equation solved for the face flux field accounting for the face channels porosity (Fig. 3).

Fig. 1

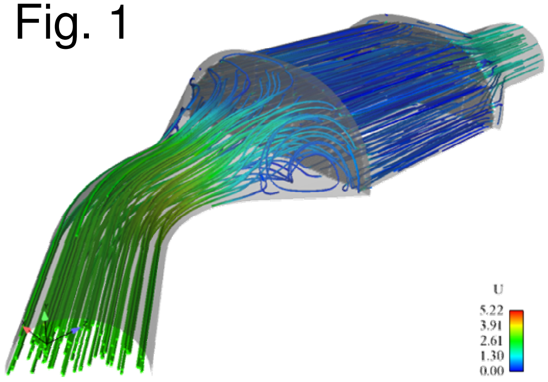


Fig. 2

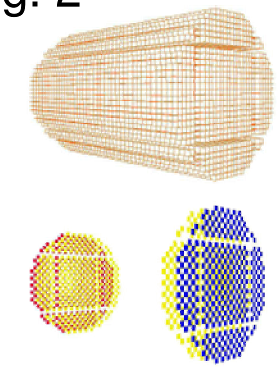
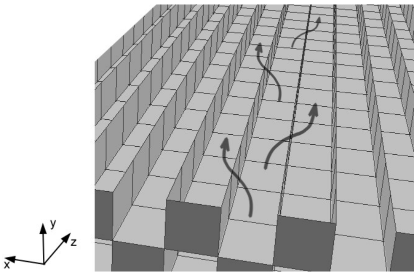


Fig. 3



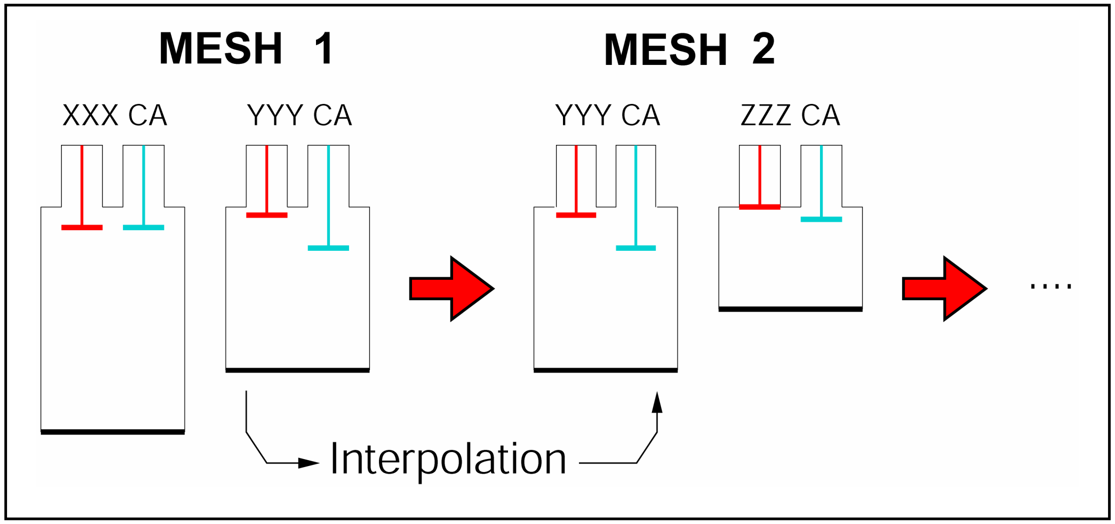
libEngine

Diesel spray combustion modeling

- Mesh management: automatic mesh motion, adaptive local mesh refinement.
- Development of new spray sub-models: atomization, droplet-wall interaction models
- Modeling liquid film formation and evolution
- Development of combustion models:
  - TITC (Tabulated ignition + Eddy Dissipation Model)
  - CTC (Characteristic Time-scale model)
  - PSR (Perfectly Stirred Reactor Model with complex chemistry and tabulation)

libEngine: mesh

Simulation strategies



Multiple meshes cover the engine cycle simulation:

- Each mesh is valid for a certain crank angle interval.
- Mesh motion + topology change at each time-step.
- Mesh-to-mesh interpolation by inverse, distance-weighted technique.

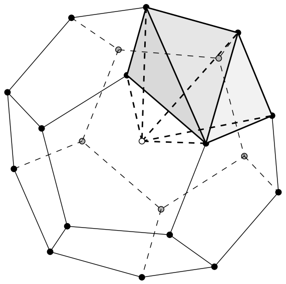
libEngine: mesh

Polyhedral, vertex based, automatic mesh motion solver

- The **Laplace equation** governs mesh motion
- Solved for the grid point velocity field **u**

Motion equation: $\nabla^2(\gamma \mathbf{u}) = 0$

New point position: $\mathbf{x}_{new} = \mathbf{x}_{old} + \mathbf{u}\Delta t$



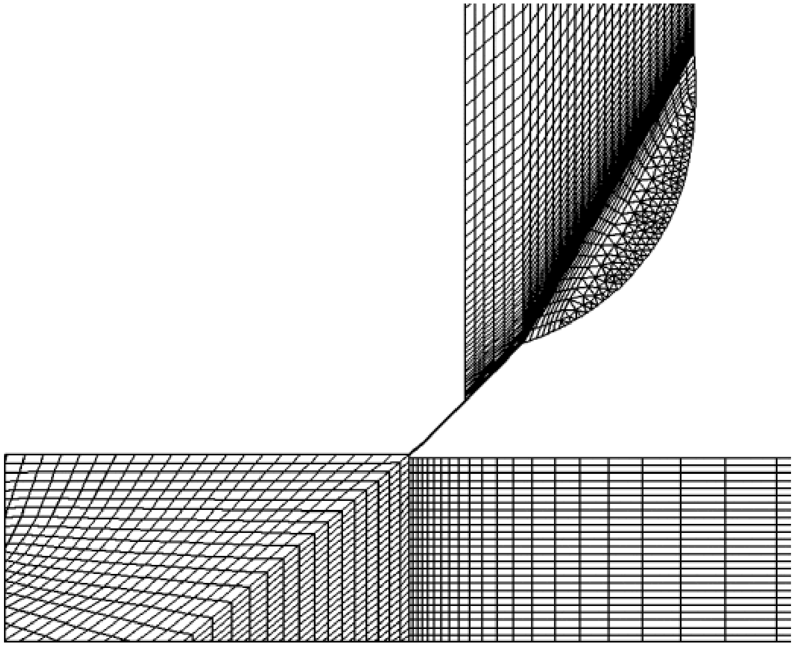
- Laplace equation solved on a finite-element decomposition of the FV mesh (*Cell decomposition*)
- Mesh validity preserved.

- Different motion boundary conditions (fixed value, fixed gradient, symmetry, periodic, …) available to accommodate mesh motion for the most complex geometries

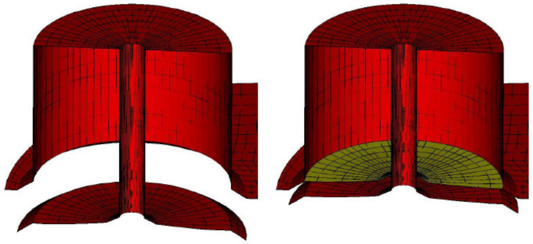
libEngine: mesh

Dynamic mesh management (Topological changes)

Dynamic mesh layering + sliding interface



Attach/detach boundary



ALGORITHM

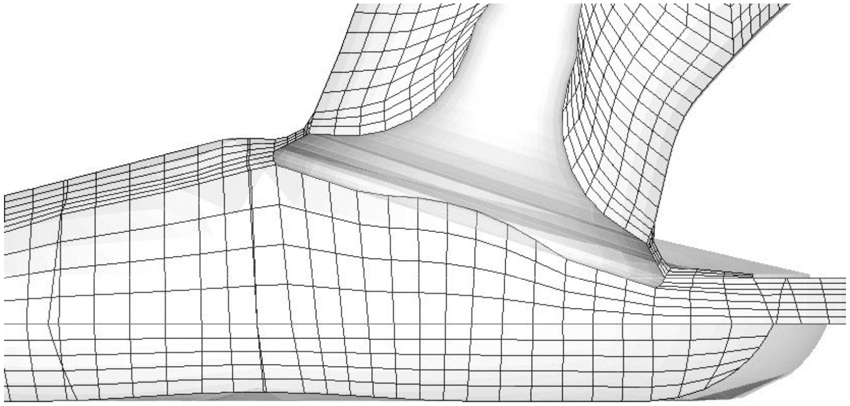
At each time step:

1) Sliding interfaces detached
2) Layers added or removed
3) Points motion
4) Sliding interfaces re-attached

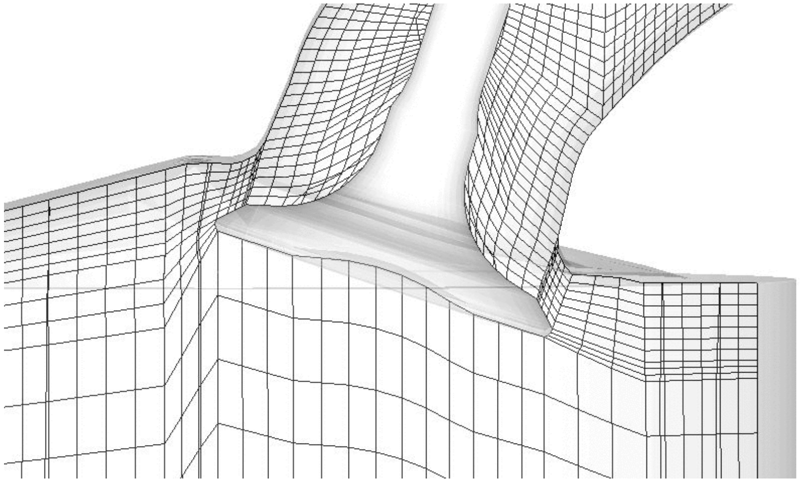
libEngine: mesh

Mesh motion: deforming mesh

Piston-valve interaction



Valve closure time

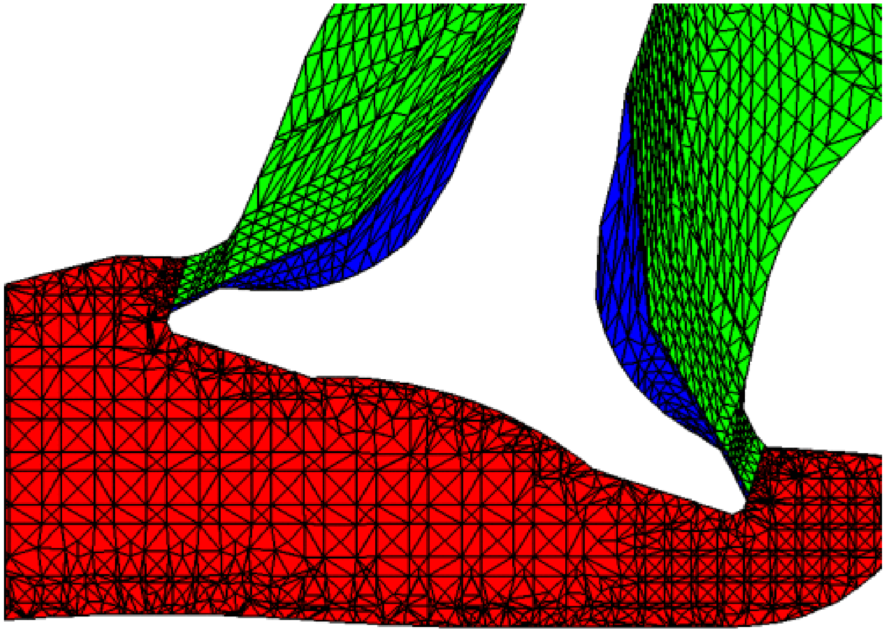


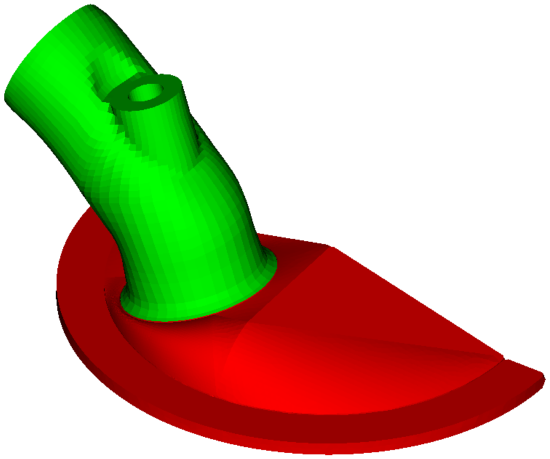
- Grid generated with ICEM-CFD – fully hexahedral.
- Mesh quality preserved during motion.
- Possibility to specify the mesh motion “a priori” for certain mesh regions, to control the mesh deformation where a high quality is needed.

libEngine: mesh

Motorcycle SI engine

Bore	72 mm
Stroke	60 mm
Compr. ratio	~ 11

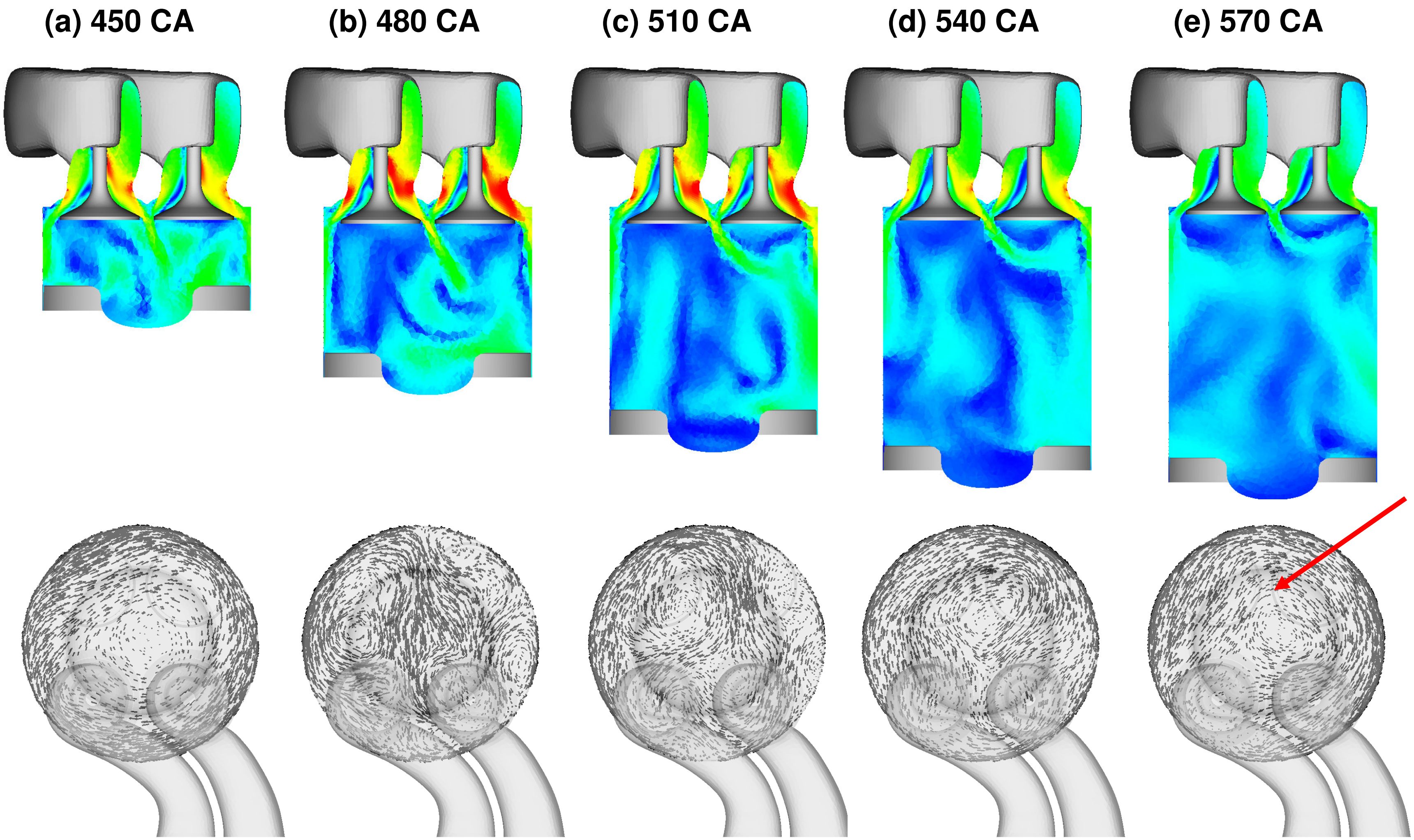




Combined operation of sliding interfaces and dynamic mesh layering on a canted-valve engine.

libEngine: mesh

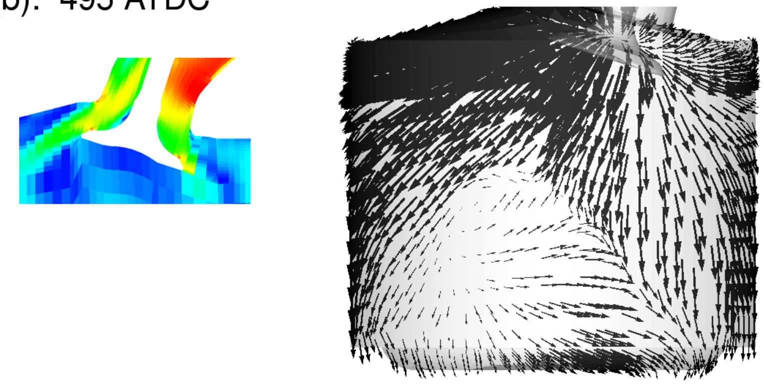
Intake stroke simulation in a Diesel Engine



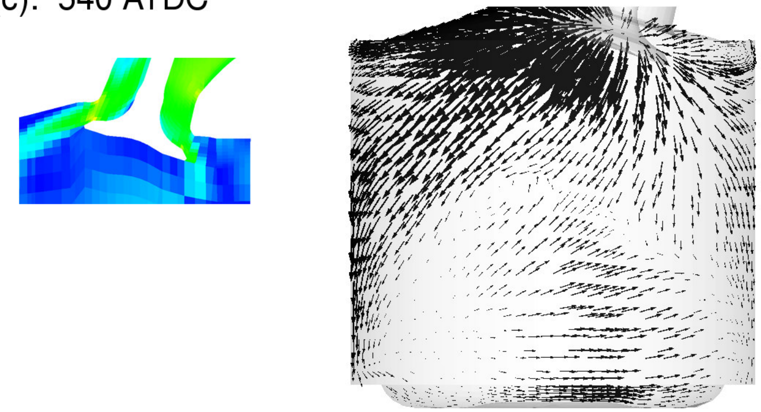
libEngine: mesh

Intake stroke simulation in a SI Engine

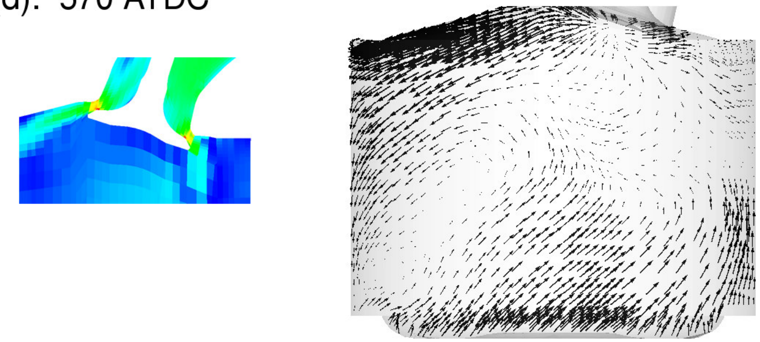
(b): 495 ATDC



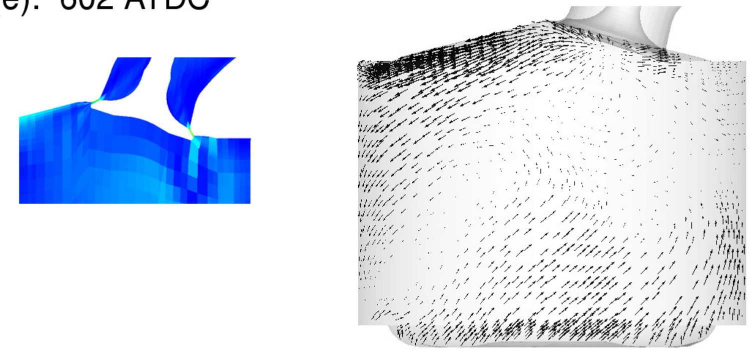
(c): 540 ATDC



(d): 570 ATDC

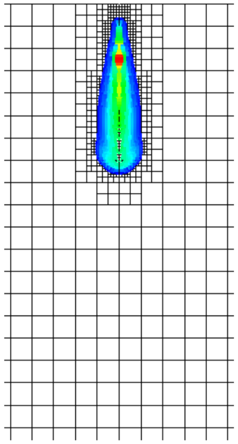


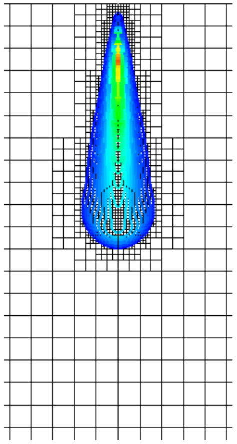
(e): 602 ATDC

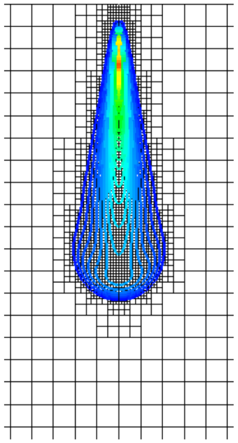


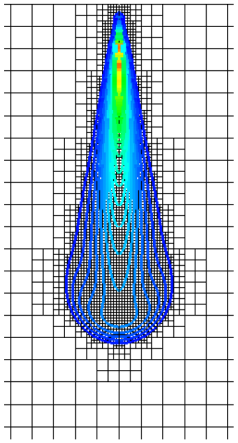
libEngine: mesh and spray

Adaptive local mesh refinement


(a) t = 0.5 ms


(b) t = 1.0 ms


(c) t = 1.5 ms


(d) t = 2.0 ms

- To reduce the computational time and keep the same accuracy of fine meshes.
- The mesh is refined if a user-specified REFINEMENT CRITERIUM is satisfied:

$$F_{min} \leq F \leq F_{max}$$

- Supports hexahedral mesh topology and mesh motion. Possibility to simulate real geometries.

libEngine: spray

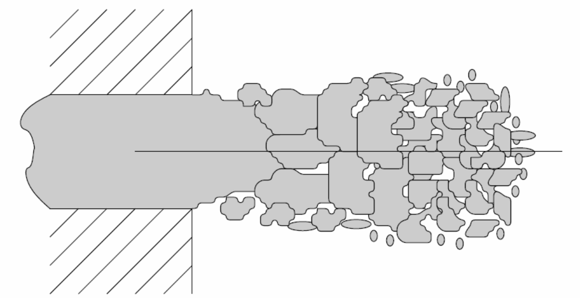
- Implementation of new spray sub-models:
  - Atomization
    - Modified Huh-Gosman (collaboration with Prof. G. Bianchi e Dr. F. Brusiani from Università degli Studi di Bologna).
    - Wave
    - Wave-KHRT
  - Injection
  - Droplet-wall interaction

libEngine: spray

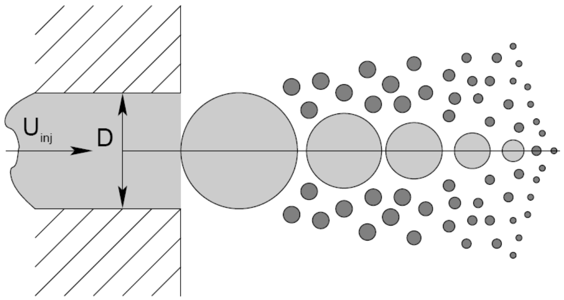
Modified Huh-Gosman model

- Parent parcels, representing the liquid fuel core are injected into the computational mesh.
- Dormant liquid core (no evaporation, drag and heat transfer)
- The parent parcel diameter is reduced due to primary breakup:
  - Diameter reduction.
  - Secondary droplets are stripped from the liquid core.

Liquid jet atomization (real)



Liquid jet atomization (model)



libEngine: spray

Modified Huh-Gosman model

- Reduction of primary droplet diameter and spray cone angle depend on a typical breakup time and length:

$$\frac{dD}{dt} = -C_5 \frac{L_a}{\tau_a} \qquad \tan\left(\frac{\theta}{2}\right) = \frac{L_a / \tau_a}{U}$$

- New parcels are created depending on the ration between the amount of stripped mass from the primary droplet and its mass.

$$\frac{m_s}{m_d} \geq s,\ \ 0.01 \leq s \leq 0.1$$

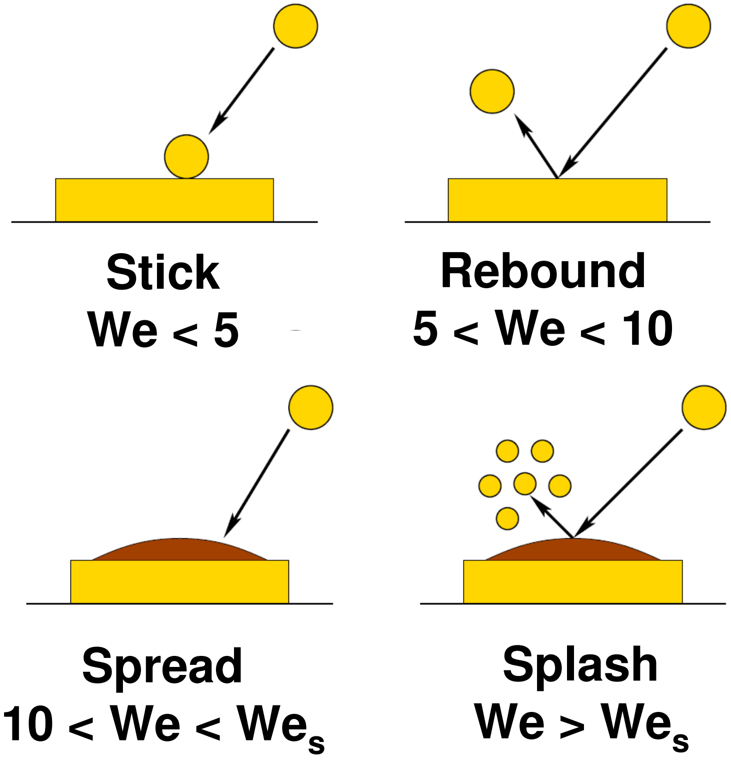
- Diameter of secondary droplets is derived from DNS calculations of liquid jet breakup under different operating conditions (nozzle Reynolds number, ambient density).

libEngine: spray

Droplet-wall interaction model

- Impinging regime depends on the **Weber** number:

$$We = \frac{\rho \left(\vec{\mathbf{V}}_{\mathbf{p}} \vec{\mathbf{n}}_{\mathbf{w}} \right) d_0}{\sigma}$$



Stick
$We < 5$

Rebound
$5 < We < 10$

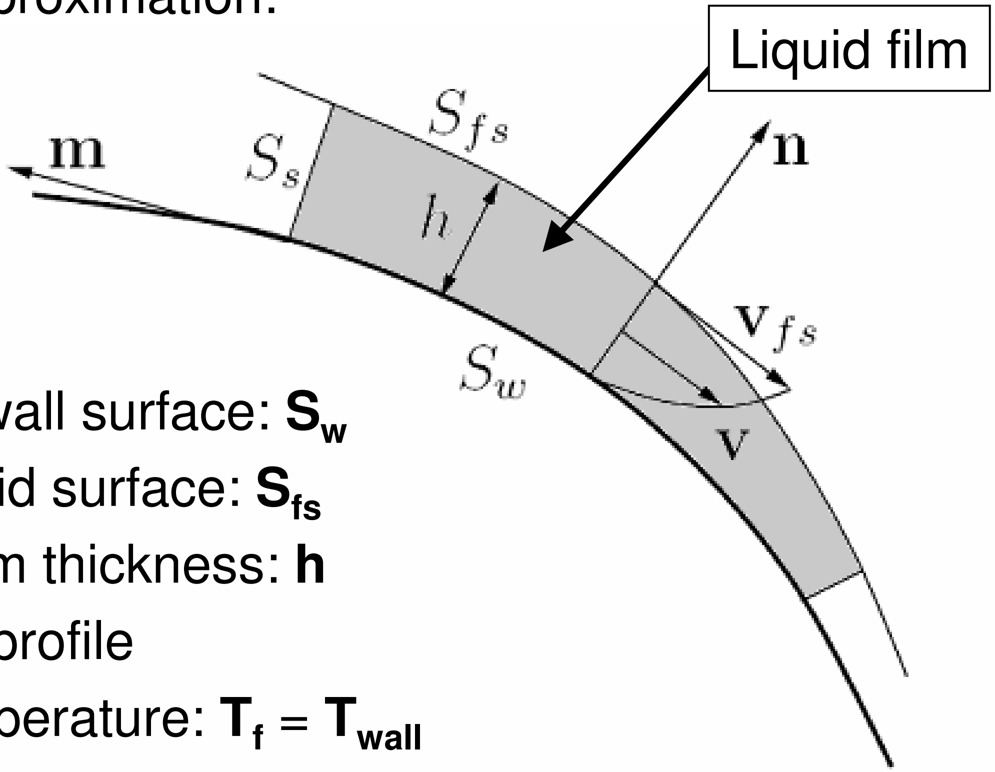
Spread
$10 < We < We_s$

Splash
$We > We_s$

- ➢ Exchange of mass, momentum and energy between **the fuel spray** and **the liquid film**.
- ➢ Consequent formation of a liquid fuel film.
- ➢ Originally proposed by Stanton and Rutland (SAE-980132).

libEngine: spray-wall interaction

- Approach proposed by Bai and Gosman (SAE-960626). Developed in collaboration with Dr. Z. Tukovic and Dr. H. Jasak.
- Simulation of the fuel film flow on an arbitrary configuration.
- Thin film approximation:

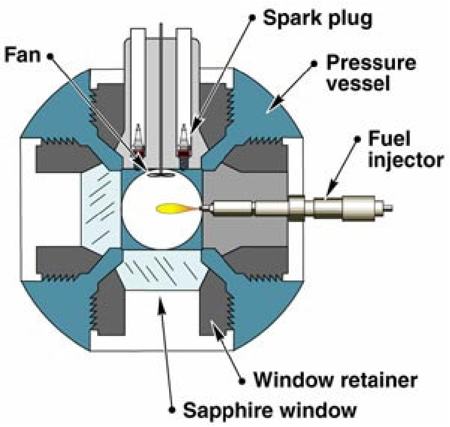


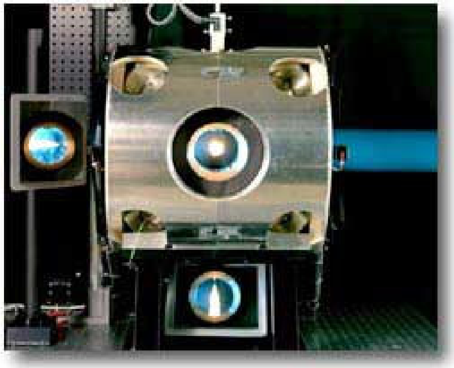
  - Curved wall surface: $\mathbf{S_w}$
  - Free liquid surface: $\mathbf{S_{fs}}$
  - Liquid film thickness: **h**
  - Velocity profile
  - Film temperature: $\mathbf{T_f = T_{wall}}$

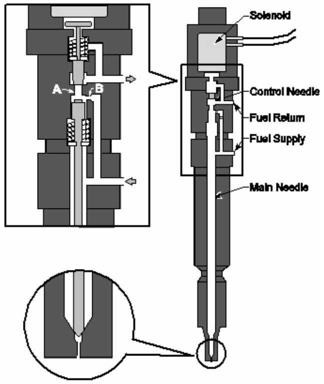
libEngine: spray

Evaporating spray at constant-volume conditions

- SANDIA combustion chamber (www.ca.sandia.gov/ecn)
- Experimental data of injection profile
- Injection pressure 1500 bar
- Non-reacting conditions (100% N_2)
- *n-heptane* fuel, ambient density 14.8 kg/m^3

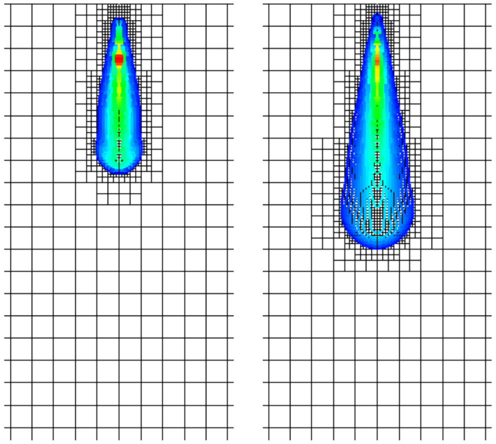




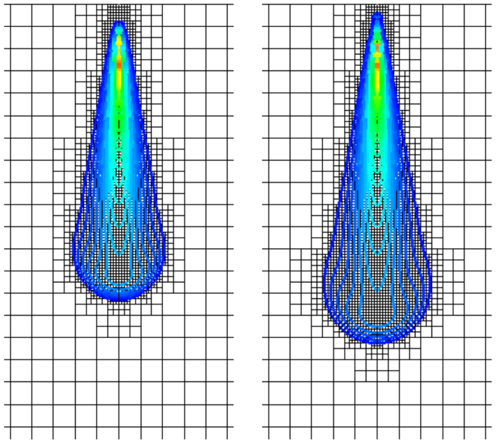


libEngine: spray

Evaporating spray at constant-volume conditions

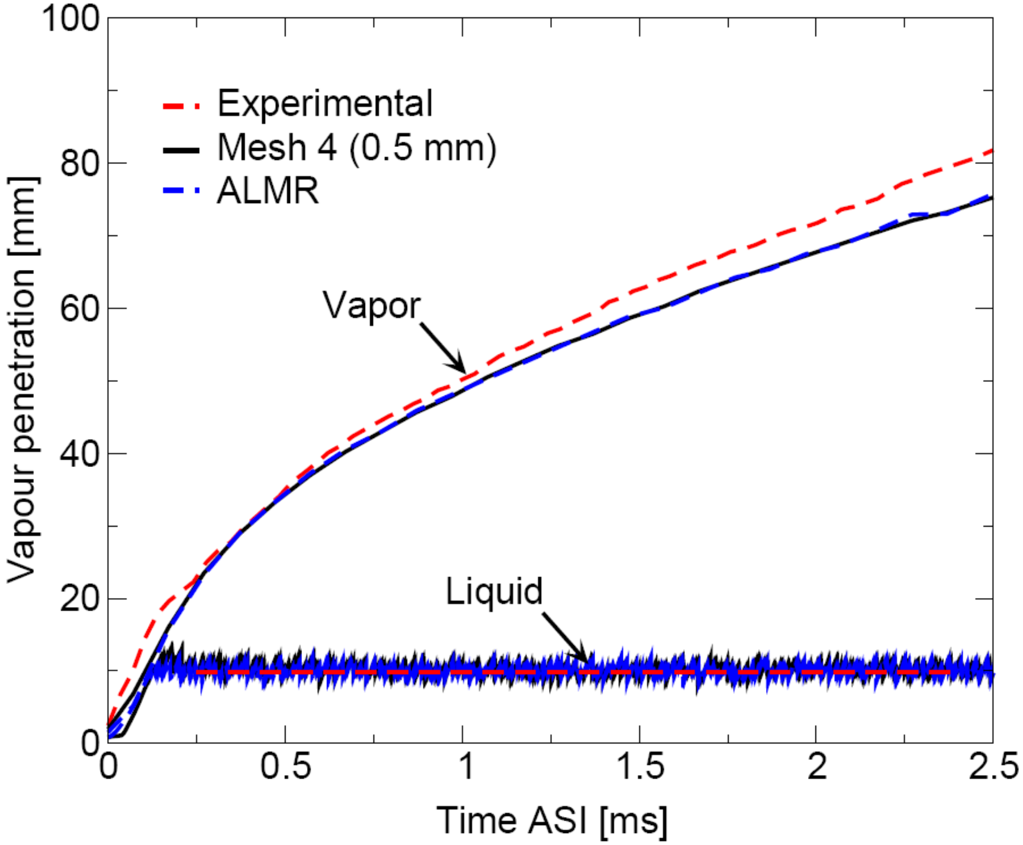


(a) t = 0.5 ms (b) t = 1.0 ms



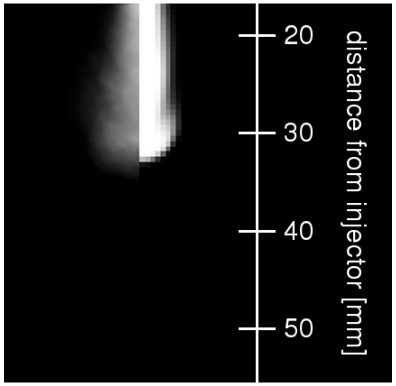
(c) t = 1.5 ms (d) t = 2.0 ms

Liquid and vapour penetration

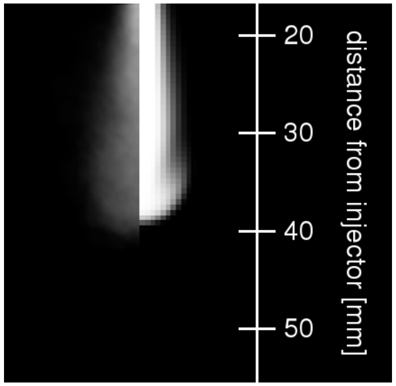


libEngine: spray

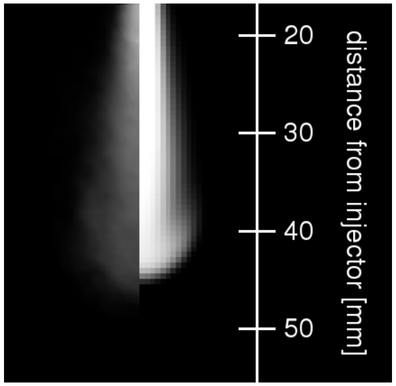
Comparison with
Rayleigh-Scattering Images



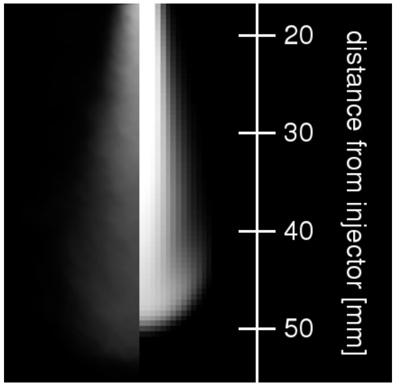
t = 0.43 ms



t = 0.68 ms

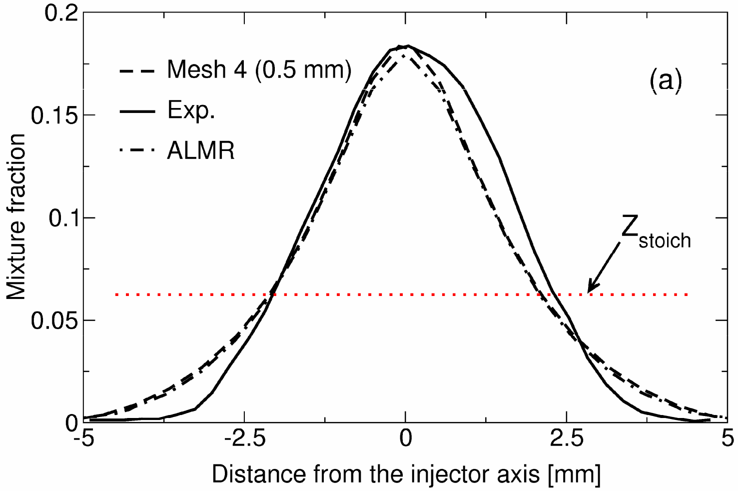


t = 0.90 ms

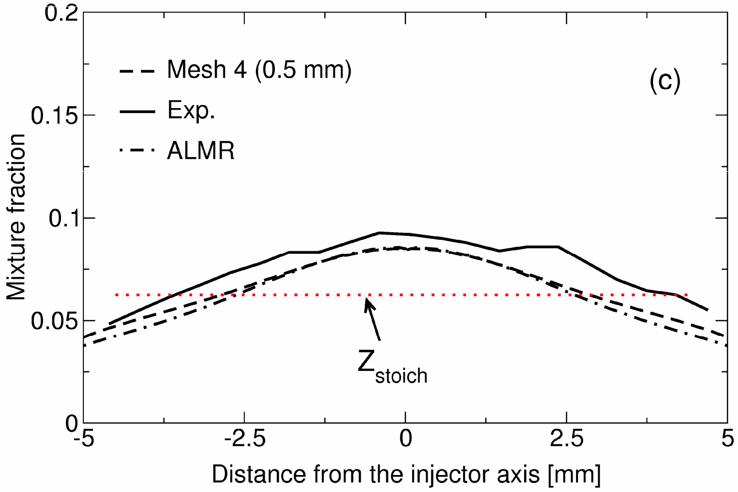


t = 1.13 ms

Time = 0.90 ms ASI, d = 20 mm



Time = 0.90 ms ASI, d = 40 mm



libEngine: spray

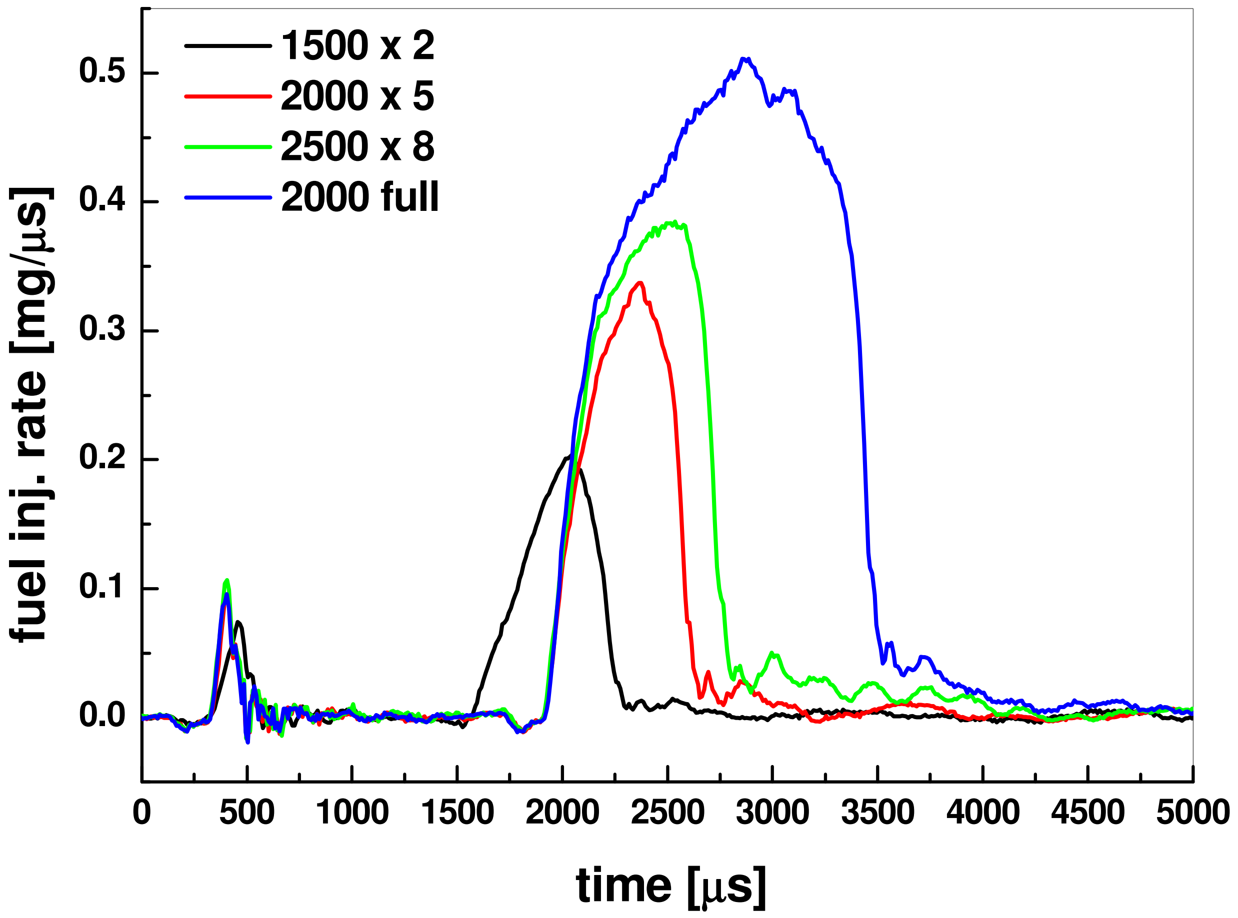
Non-evaporating spray at constant-volume conditions with multiple injections.

- Model verified at different ambient conditions with different injection strategies (to be published at SAE World Congress 2010).

Strategy	Q_{pilot} [mm^3/stroke]	Q_{tot} [mm^3/stroke]	Ambient density [kg/m^3]
1500 x 2	1.04	10.94	16.3
2000 x 5	0.93	20.01	18.6
2000 full	0.93	73.19	33.6
2500 x 8	1.04	29.67	23.9

libEngine: spray

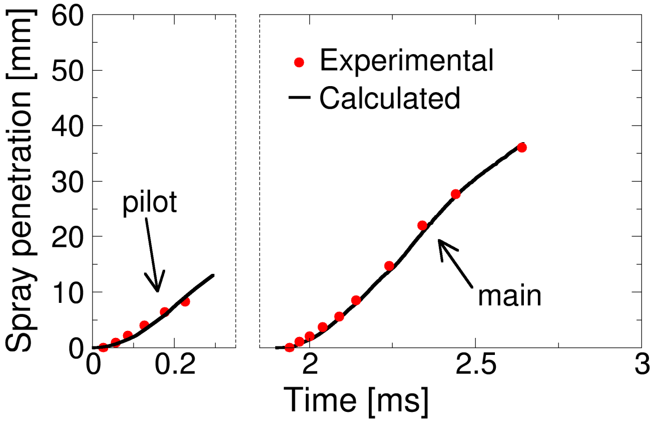
Non-evaporating spray at constant-volume conditions with multiple injections.



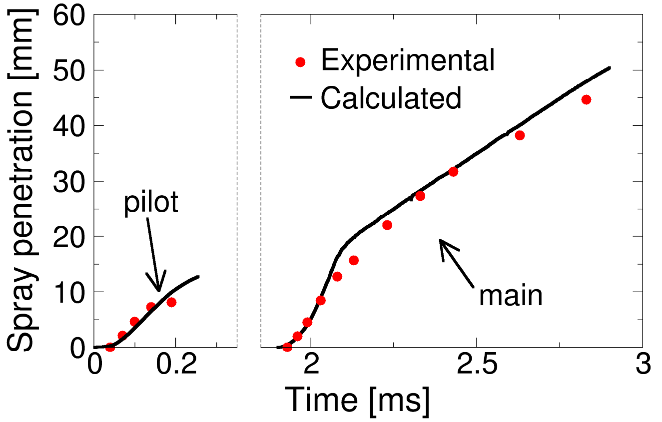
libEngine: spray

Non-evaporating spray at constant-volume conditions with multiple injections.

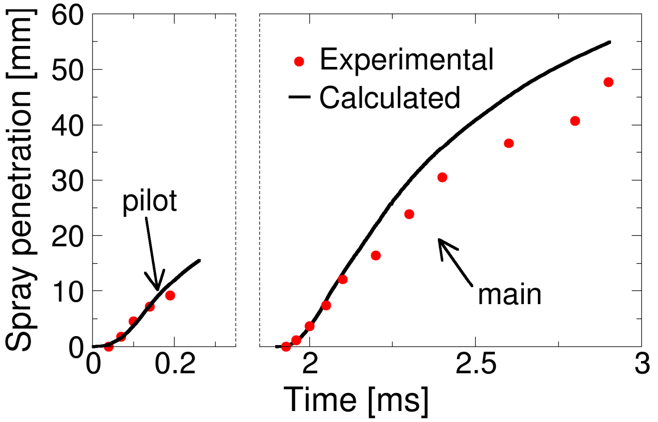
(a) Strategy 1500 x 2, ρ_{amb}=16.3 kg/m^3



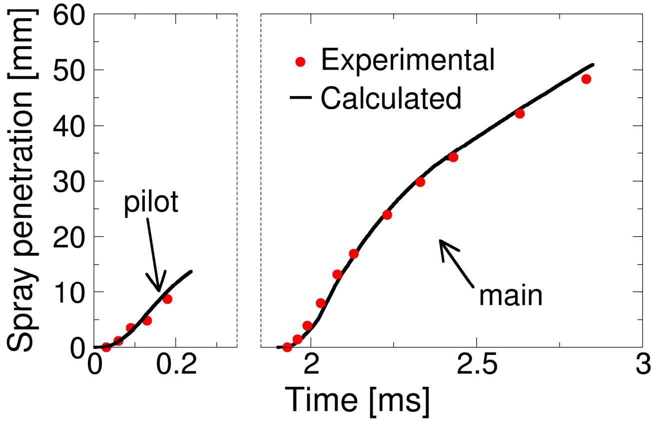
(a) Strategy 2000-full, ρ_{amb}=33.6 kg/m^3



(b) Strategy 2000 x 5, ρ_{amb}=18.6 kg/m^3

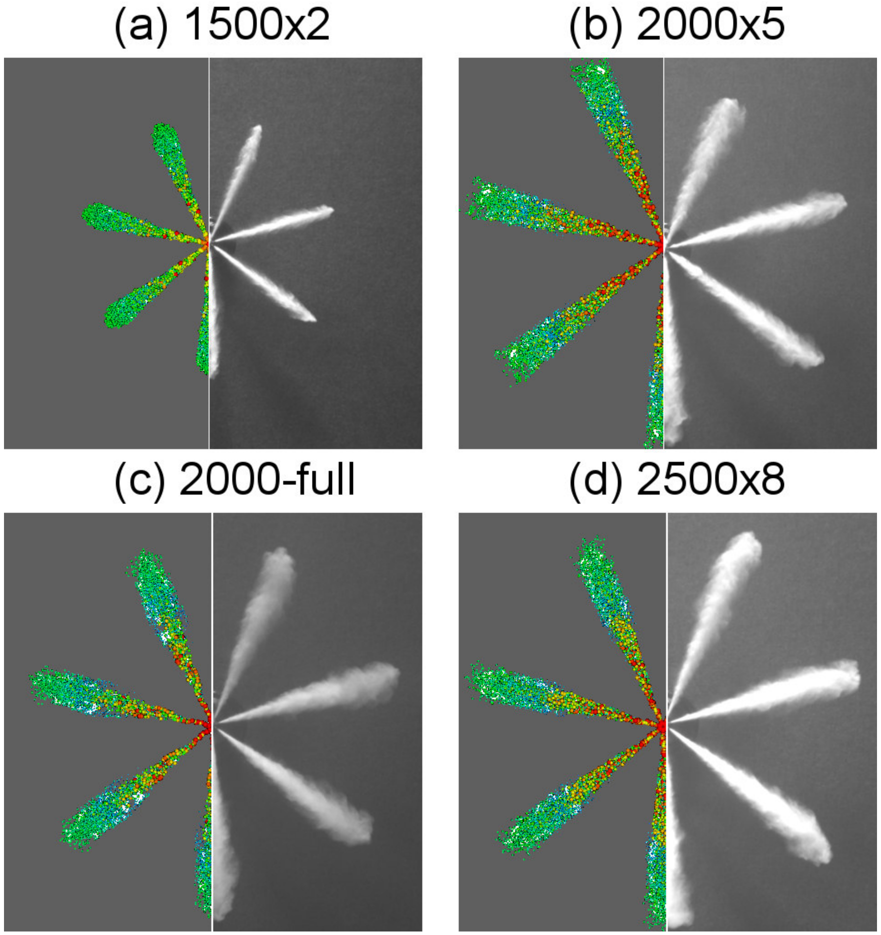


(b) Strategy 2500 x 8, ρ_{amb}=23.9 kg/m^3



libEngine: spray

Non-evaporating spray at constant-volume conditions with multiple injections.



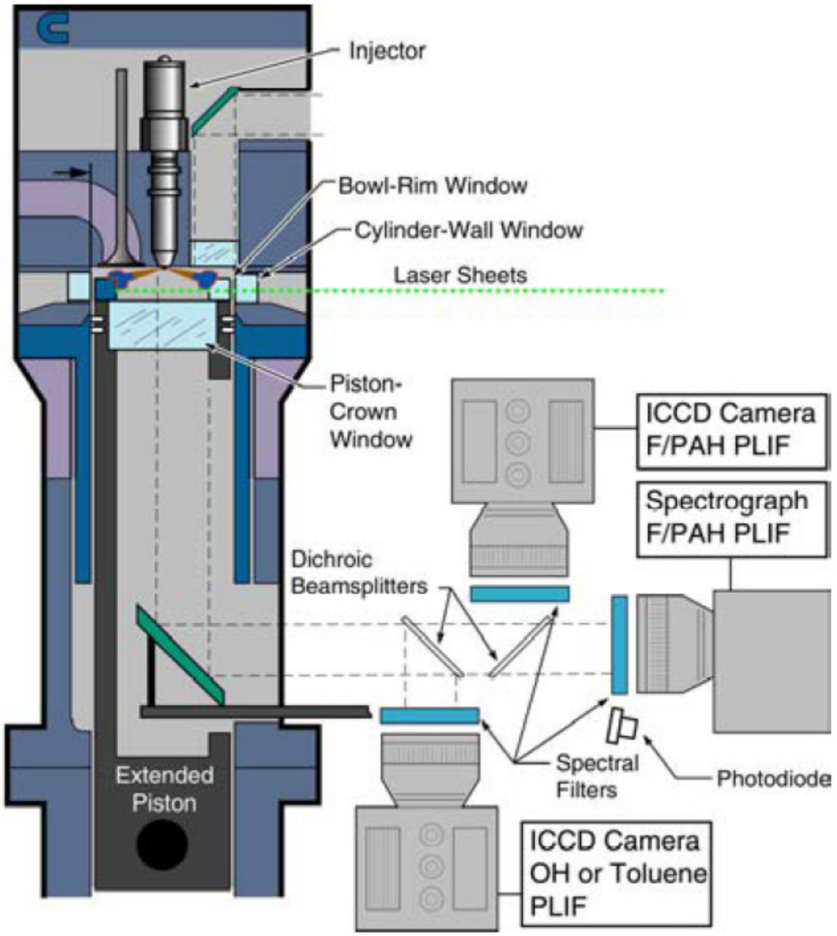
Computed results in good agreement with experimental data:

- Liquid length for both the pilot and the main injections
- Spray shape and cone angles.

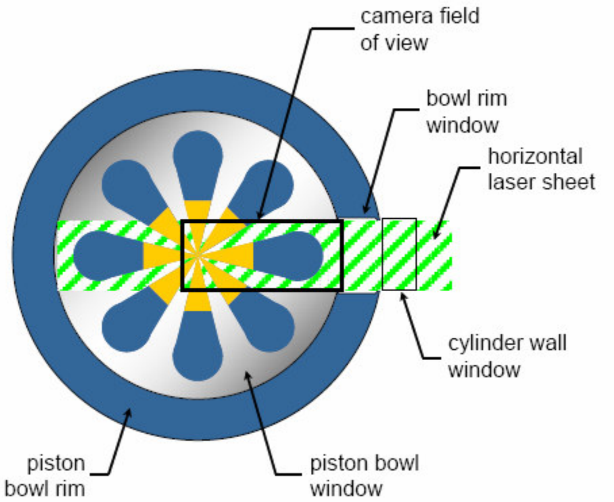
Experimental data from:
Dr. A. Montanaro and Dr. L. Allocca
(CNR-Istituto Motori, Naples)

libEngine: spray

Evaporating spray in an optical engine



Swirl ratio	0.5
Bore	139.7 mm
Stroke	152.4 mm
Compression Ratio	16.1 (12.1)
Intake pressure	2 bar
Fuel	PRF29



libEngine: spray

Evaporating spray in an optical engine

Operating conditions

Operation	Non-reacting
Engine speed, RPM	1200
IMEP, kPa	400
Injected fuel mass, mg	56
Injection duration, CAD	6.75
SOI, ºATDC	0
Intake oxygen [%]	0
Equivalent EGR [%]	100
Equivalence ratio	0
Intake Temperature [ºC]	72
Intake pressure [bar]	206

MESH MANAGEMENT

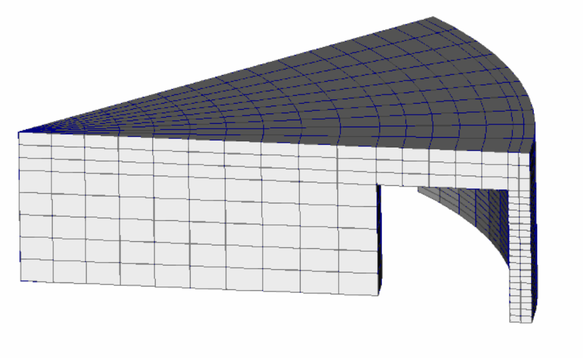
- Compression stroke:
  - ✓ Layered coarse mesh + layer addition removal
- Injection and air-fuel mixture formation:
  - ✓ Coarse mesh with adaptive local mesh refinement.

libEngine: spray

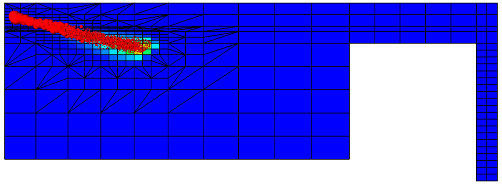
Evaporating spray in an optical engine

Fuel/air mixture formation during the injection phase with adaptive local mesh refinement.

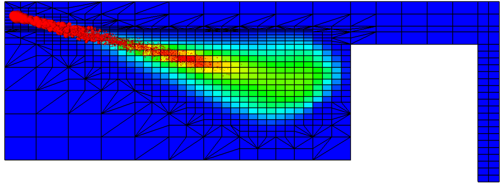
- Initial mesh: size 4 mm in the bowl region



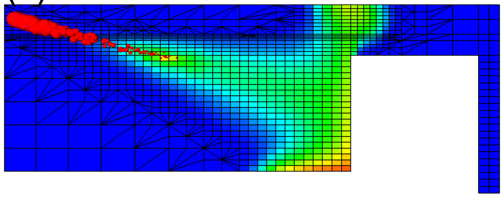
(a) 2 ATDC



(b) 5 ATDC



(c) 10 ATDC

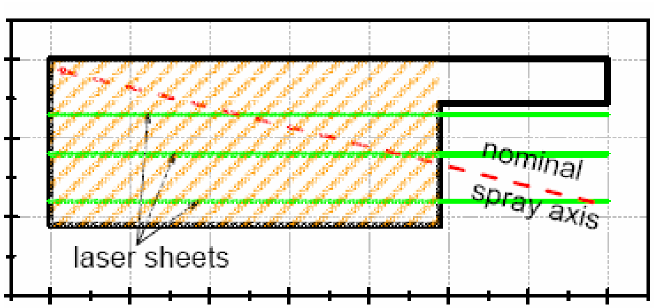


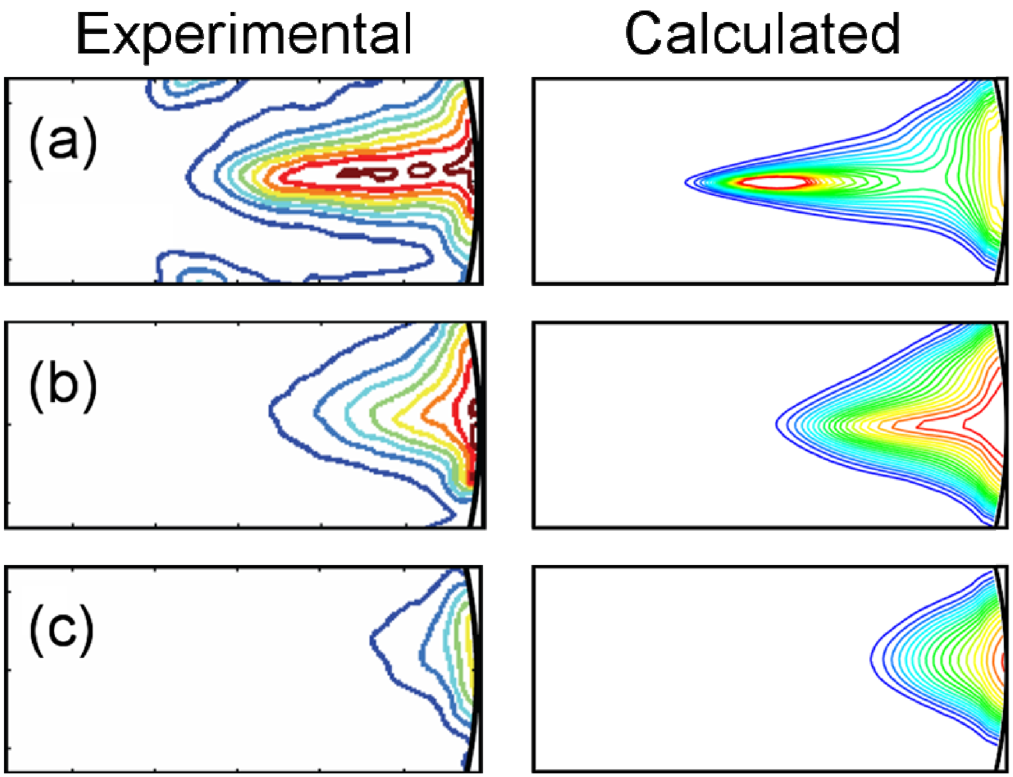
libEngine: spray

Evaporating spray in an optical engine

Comparison between experimental and computed fuel mass fraction on three different cut planes.

Time: 7 CAD ATDC





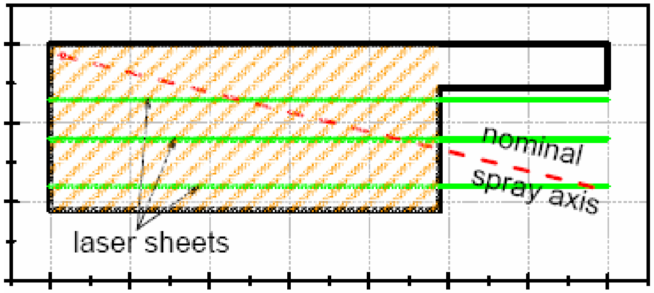
- Correct estimation of the fuel vapor distribution on the three different cut planes

libEngine: spray

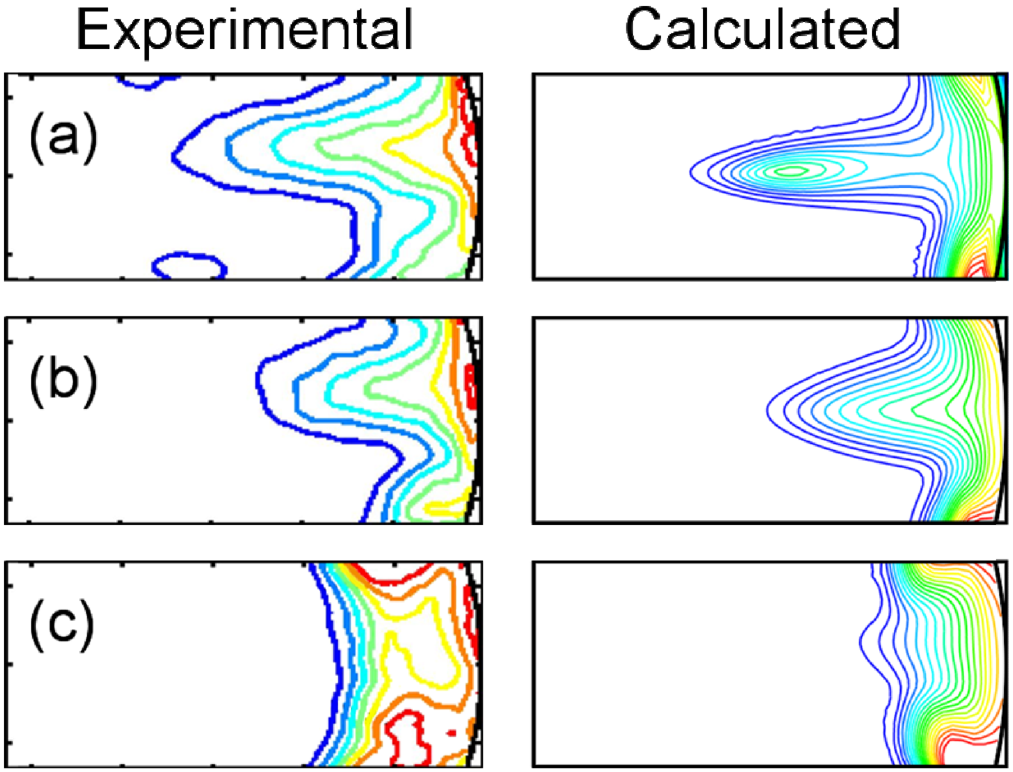
Evaporating spray in an optical engine

Comparison between experimental and computed fuel mass fraction on three different cut planes.

Time: 12 CAD ATDC

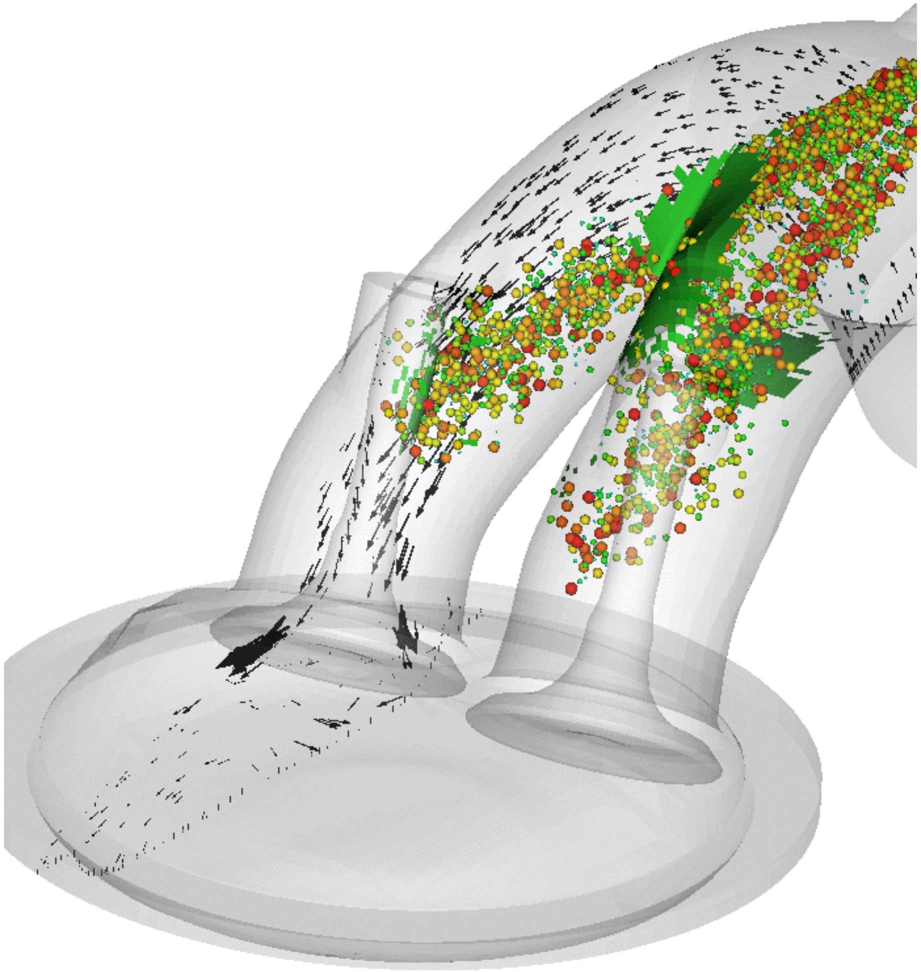


- Correct estimation of the fuel vapor distribution on the three different cut planes



libEngine: spray

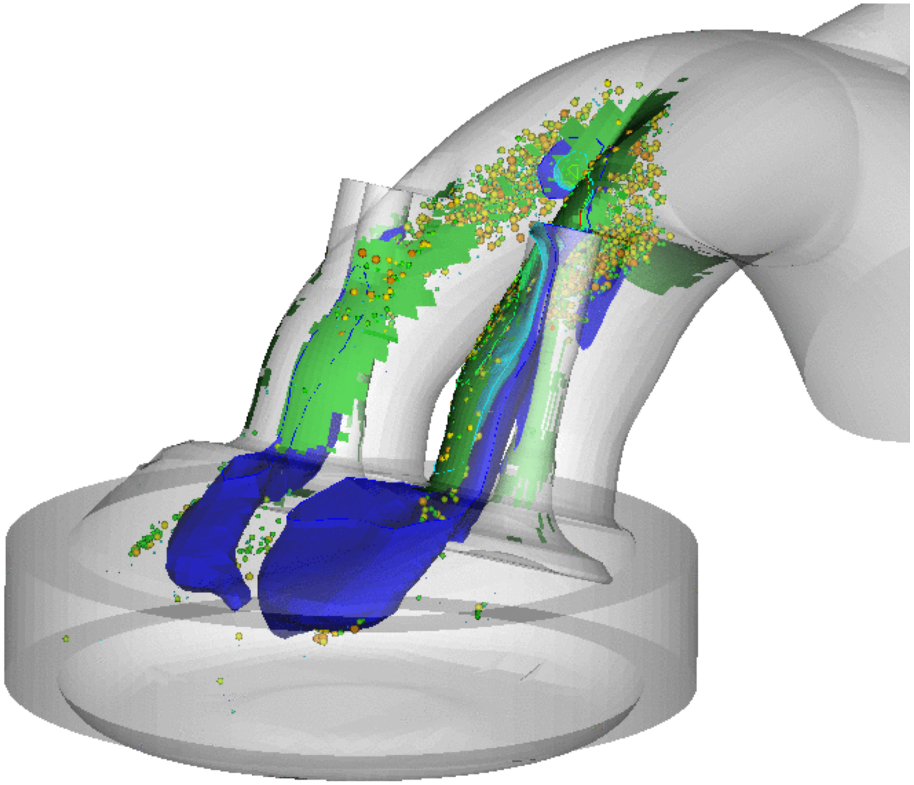
Fuel injection in a PFI engine



- Film deposition on the valves:
  - Finite area works in combination with mesh motion
- Fuel spray convected by the flow into the cylinder

libEngine: spray

Fuel injection in a PFI engine



- Isosurfaces of fuel mass fractions to understand how fuel/air mixture formation takes place:

- The fuel vapor mainly comes from wall film.

- Computed results in agreement with a previous work carried out on the same engine (SAE 2007-24-0041)

libEngine: combustion

Objectives

- Improve the existing combustion models to provide advanced diagnostic and development tools to design and simulate Diesel engines.

- This requires to:
  - Implement the state of the art of existing combustion models on the same platform (libEngine).
  - Compare them with a series of well-documented Diesel combustion experiments.

- In this way it will be possible to develop a new generation of combustion models.

libEngine: combustion

TITC (Tabulated auto-Ignition + Turbulent Combustion)

- Four chemical species (air, fuel, products, residuals)
- The fuel reaction rate accounts for auto-ignition (*α=0*) and mixing controlled combustion (*α=1*) :

$$\dot{\omega}_F = (1-\alpha)\dot{\omega}_{F,HT} + \alpha\dot{\omega}_{F,mix}$$

- Tabulated ignition delays from detailed chemistry to estimate auto-ignition time
- **Eddy dissipation model (Magnussen)** to calculate the mixing controlled combustion phase:

$$\rho\dot{\omega}_{F,MIX} = C_{mag}\rho\frac{\varepsilon}{k}\min\left(Y_F, \frac{Y_O}{s}, \beta\frac{Y_P}{1+s}\right)$$

- Predicts both auto-ignition and flame stabilization. **Fast and reliable**.

libEngine: combustion

CTC (Characteristic Time-scale Combustion Model)

- 11 chemical species (fuel, O_2, N_2, CO, CO_2, H_2O, O, OH, NO, H, H_2)
- Auto-ignition computed by the Shell auto-ignition model (available set of constants for different fuels).
- Turbulent combustion simulated accounting for both laminar and turbulent time scales:

$$\dot{Y}_{i,TC} = -\frac{Y_i - Y_i^*}{\tau_C} \quad \text{, where} \quad \tau_C = \tau_l + f\tau_t$$

- Fast like TITC, but more accurate since it can be used to predict pollutant emissions (NO_x and soot).

libEngine: combustion

PSR (Perfectly Stirred Reactor Combustion Model)

- Known also as *KIVA-CHEMKIN* (Singh et al., SAE 2006-01-0055)
- Homogeneous mixture, no turbulence-chemistry interaction
- Detailed chemistry is used
  - Multi-component mixture support + reaction mechanism to be provided
  - ODE solvers
- Operator splitting technique
  - Separates the chemistry and the fluid-dynamics to estimate the species source terms (ODE integration):

$$Y_i^*(t+\Delta t) = Y_i(t) + \int_t^{t+\Delta t} \dot{\omega}_i \frac{W_i}{\rho}\, dt' \Longrightarrow \dot{Y}_i = \frac{Y_i^*(t+\Delta t) - Y_i(t)}{\Delta t}$$

libEngine: combustion

Validation at constant-volume conditions

Case	1	2	3	4	5	6
Ambient density [kg/m^3]	14.8	14.8	14.8	14.8	14.8	14.8
O_2 volume fraction [%]	21	15	10	21	21	21
Ambient temperature [K]	1000	1000	1000	1300	900	750
Injected Fuel Mass [mg]	17.8	17.8	18.1	18.1	17.5	17.4

Influence of ambient temperature

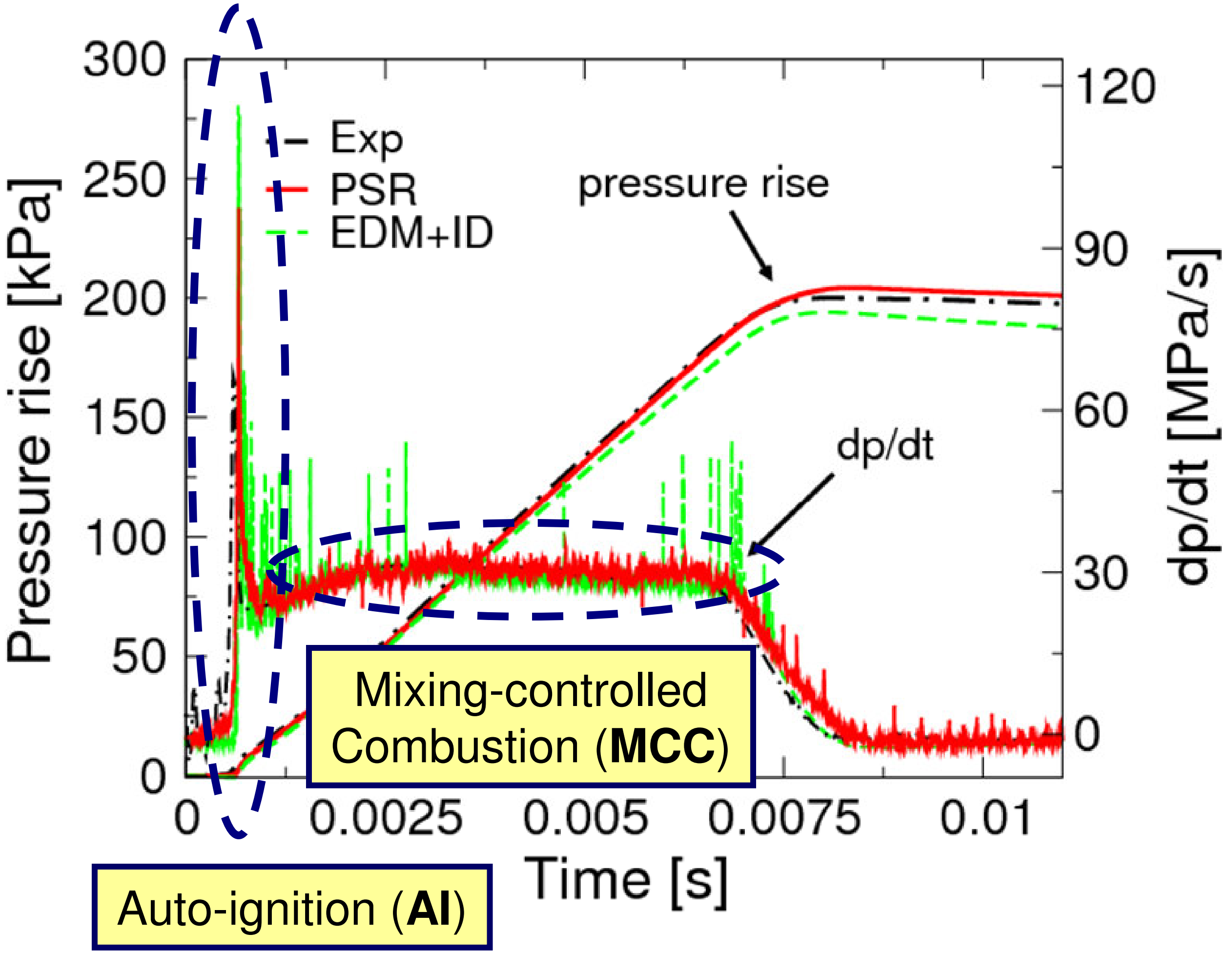
Influence of EGR

- Chemical mechanism by Patel et al.:
  - 29 species + 50 reactions (SAE 2004-01-0558).
  - Used also to derive the tabulated ignition delays.

- Other mechanisms were tested in the same conditions.

libEngine: combustion

T_{amb} = 1000 K, O_2 = 21%, ρ_{amb} = 14.8 kg/m^3 **(EGR = 0%)**

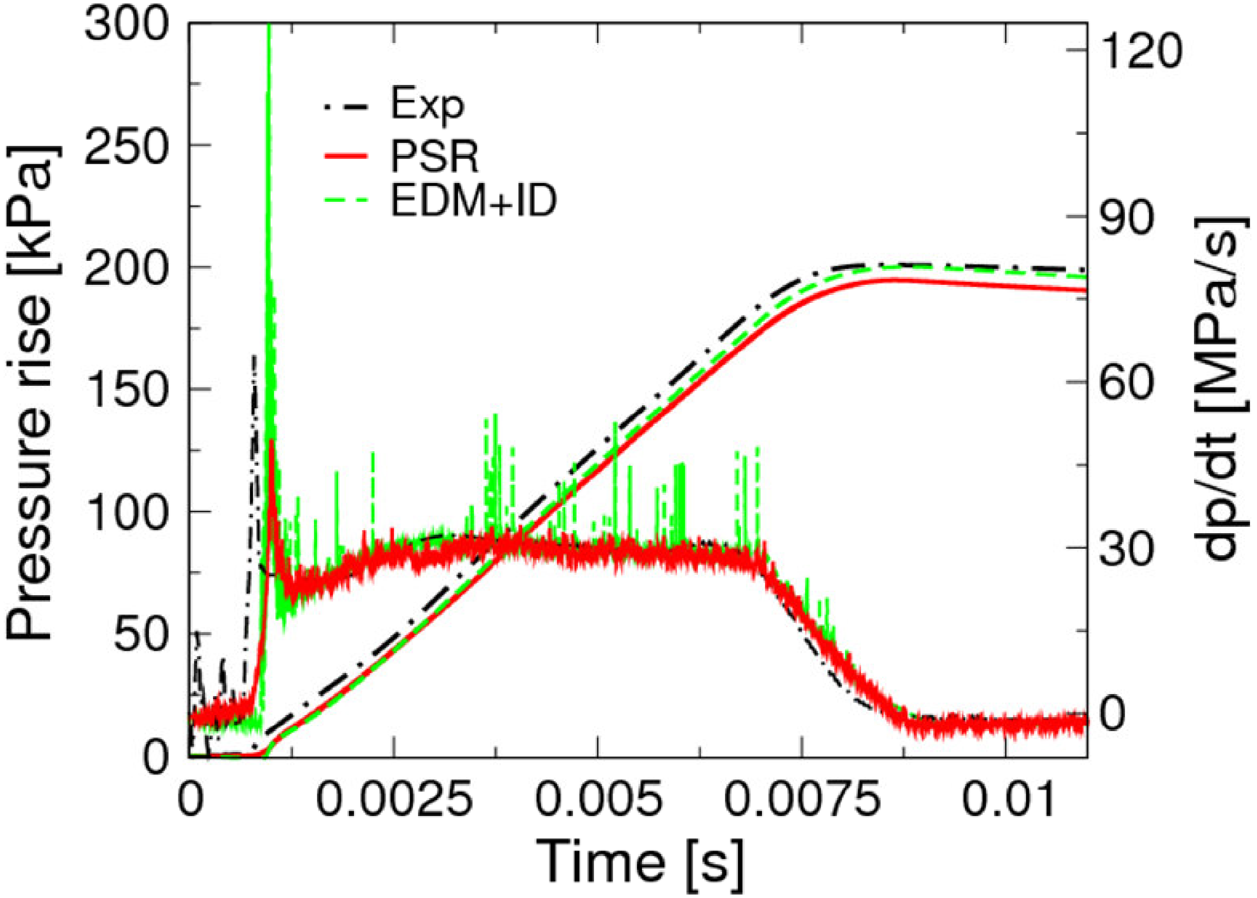


Mixing-controlled Combustion (**MCC**)

Auto-ignition (**AI**)

libEngine: combustion

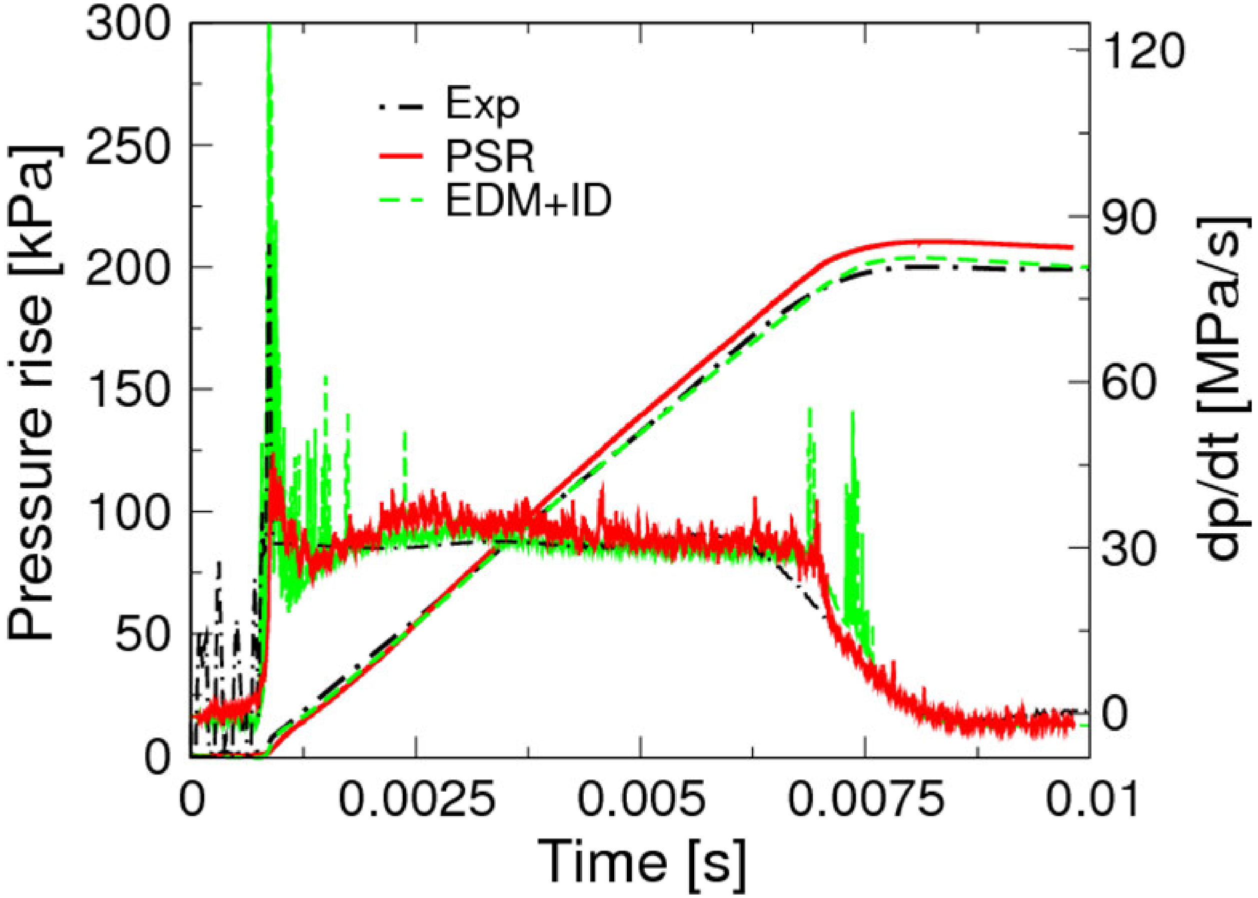
T_{amb} = 1000 K, O_2 = 15%, ρ_{amb} = 14.8 kg/m^3 **(EGR = 28%)**



libEngine: combustion

Moderate soot

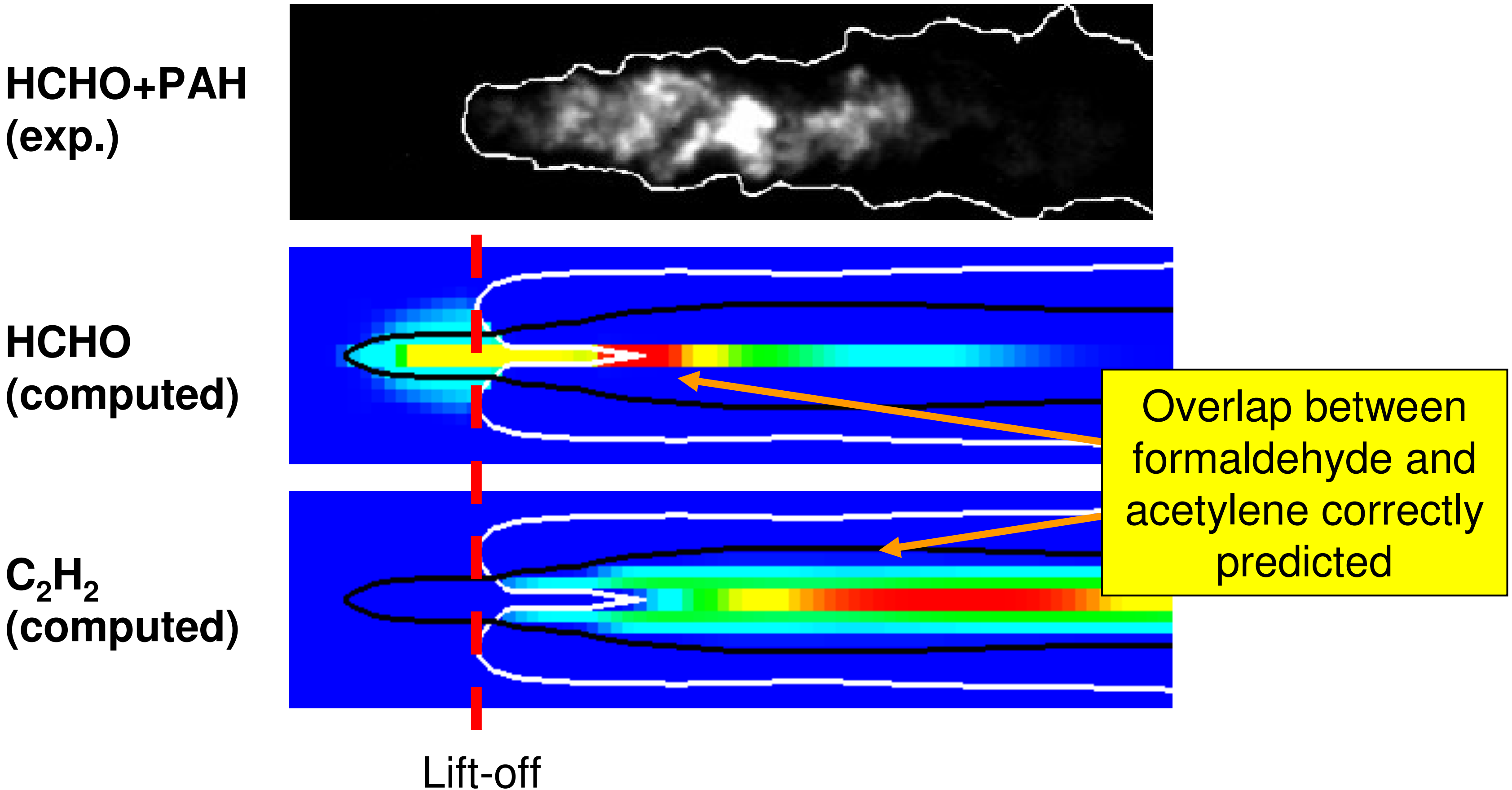
T_{amb} = 900 K, O_2 = 21%, ρ_{amb} = 14.8 kg/m^3



libEngine: combustion

Formaldehyde, PAH and soot distribution

- Moderate soot conditions (T = 1000K, O_2 = 21%)



Overlap between formaldehyde and acetylene correctly predicted

libEngine: combustion

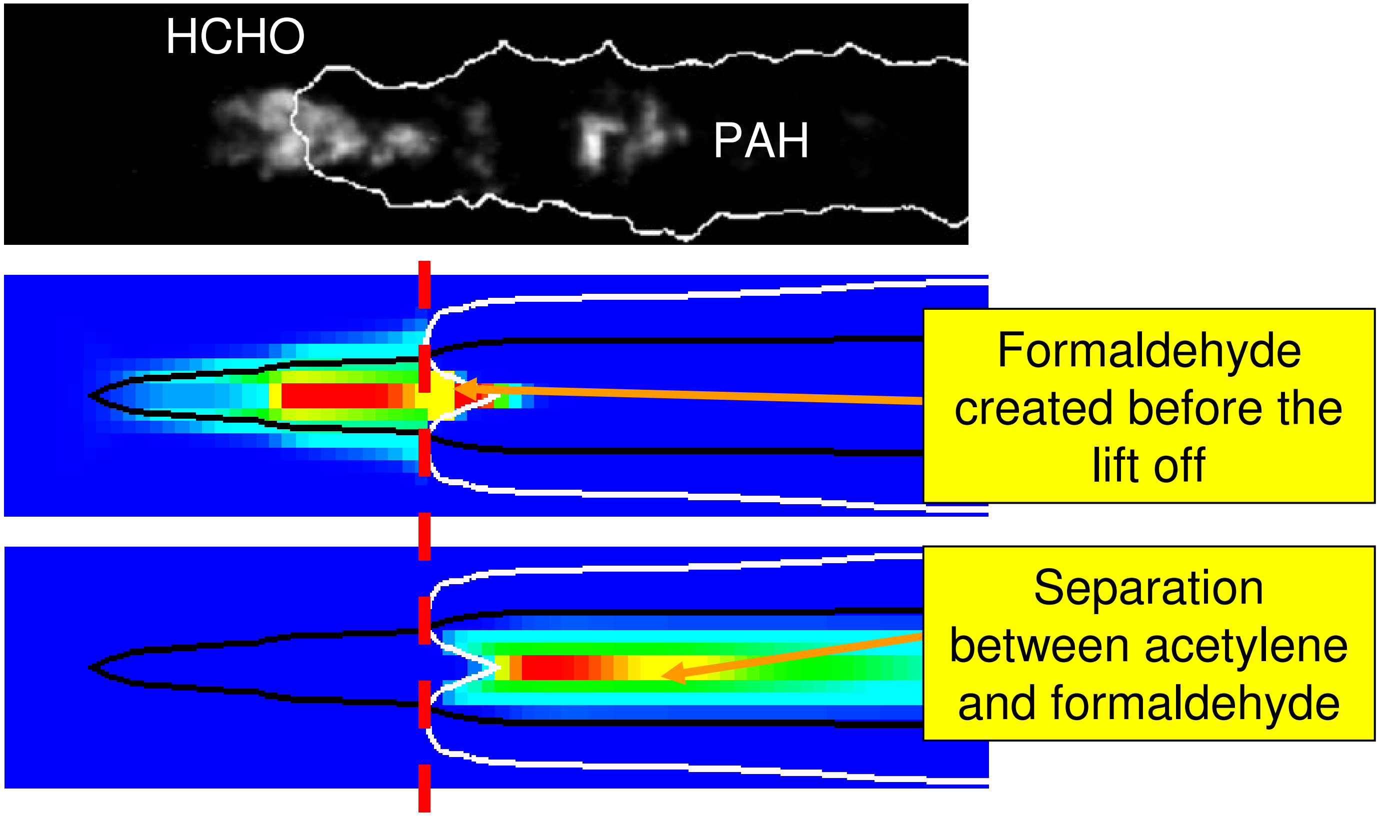
Formaldehyde, PAH and soot distribution

- Low soot conditions (T = 900K, O_2 = 21%)

HCHO+PAH (exp.)

HCHO (computed)

C_2H_2 (computed)



Formaldehyde created before the lift off

Separation between acetylene and formaldehyde

libEngine: combustion

Validation in internal combustion engine simulations

- All the three models are currently applied and verified simulating full-load conditions.
- A comprehensive validation is performed in this weeks considering:
  - Four different engine geometries (passenger car engines, heavy duty diesel engine, two-stroke diesel engine).
  - Different injection strategies (main, pilot+main, pre+pilot+main)
  - Different EGR rates (0-30%)
- The validation will carried out in terms of:
  - In-cylinder pressure profile and heat release rate.
  - Pollutant emission (NO_x and soot)

- …and presented at the 4th OpenFOAM Workshop (Goteborg, 2009)

libEngine: combustion

What to do?

- TITC – CTC: very fast, reliable models. They can be used mainly for industrial calculations and to simulate conventional diesel combustion.
- PSR: very promising model (auto-ignition, pollutant formation, flame structure), but very slow because of detailed chemistry integration. Solutions:
  - Parallelization of chemistry integration
  - Combination of in-situ adaptive tabulation (ISAT) and dynamic adaptive chemistry (DAC) → TDAC.

libEngine: combustion

TDAC (Tabulated dynamic adaptive chemistry)

- ISAT: In-situ adaptive tabulation of the reaction mapping for a species array. The complete ISAT is used including the mapping gradient matrix.

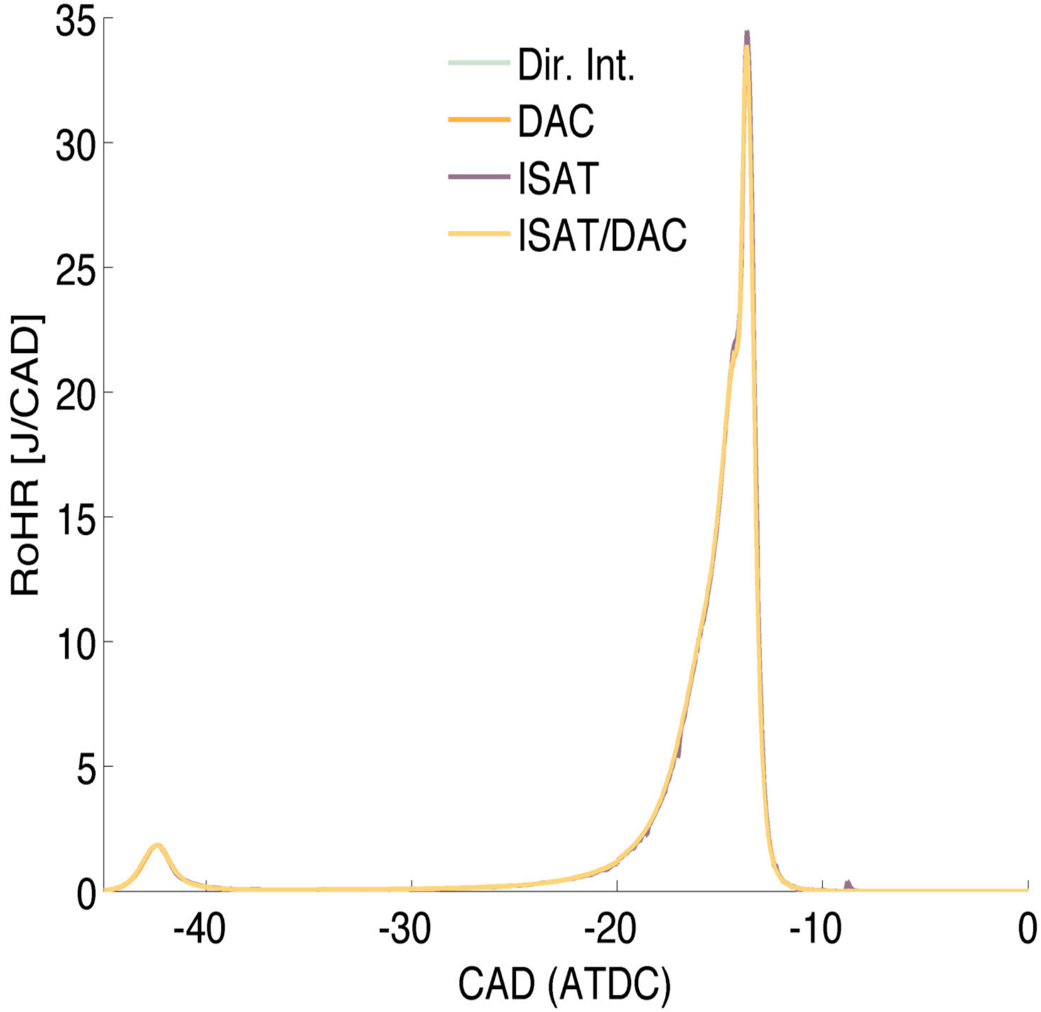
$$\mathbf{R}\left(\mathbf{Y}^{q}\right)=\mathbf{R}\left(\mathbf{Y}^{0}\right)+\frac{\partial \mathbf{R}}{\partial \mathbf{Y}}\left(\mathbf{Y}^{q}-\mathbf{Y}^{0}\right)$$

- DAC (dynamic adaptive chemistry): a detailed chemical mechanism is reduced in each computational cell involving only the significant reactions and species.
- The corresponding ODE system is calculated only for the relevant species and accounting for the relevant reactions.

libEngine: combustion

TDAC (Tabulated dynamic adaptive chemistry)

HCCI combustion simulated with n-heptane «reduced» mechanism from LLNL: 159 species and 770 reactions



libEngine: combustion

TDAC (Tabulated dynamic adaptive chemistry)

- Diesel-like combustion calculation (2D non-premixed flame)

	Direct integration	DAC	ISAT	ISAT+DAC
Speed-up factor	1	2.5	2.5	**5**

- HCCI combustion calculation

	Direct integration	DAC	ISAT	ISAT+DAC
Speed-up factor	1	3	18	**26**

Internal Combustion Engine Group

Thanks for your attention!