

# LES Simulations in a Lean SI Optical Engine Using Thickened Flame Model

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UNIVERSITÀ DEGLI STUDI  
DI PERUGIA

# Lean combustion and stability

Large-Eddy simulations (LES) are becoming an engineering tool for studying internal combustion engines (ICE)



able to capture cycle-to-cycle variability resolving most of the turbulent flow structures

ICEs can operate under lean combustion conditions to maximize efficiency



instabilities associated with lean combustion may cause problems, (excessive levels of cycle-to-cycle variability or even misfires)

In this context, the interaction between the igniter and the flow field is a fundamental parameter that affect ignition stability and how combustion takes place and develops

# Outline

1. Experimental Setup
  - Optical access SI engine
  - Ignition systems tested in Perugia University
2. CFD Model Setup
3. TFM combustion model
  - Why TFM?
  - Flame sensor
  - Thickening option and AMR
  - Efficiency function
  - Effect of the calibration parameters
4. Cycle to cycle variability prediction
  - TFM 3D output
  - Mass fraction burned at different  $\lambda$
  - Flame comparison at different  $\lambda$
5. Conclusions and next steps

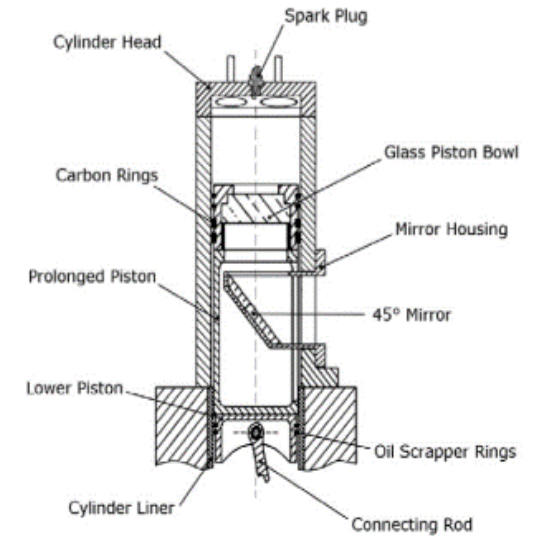
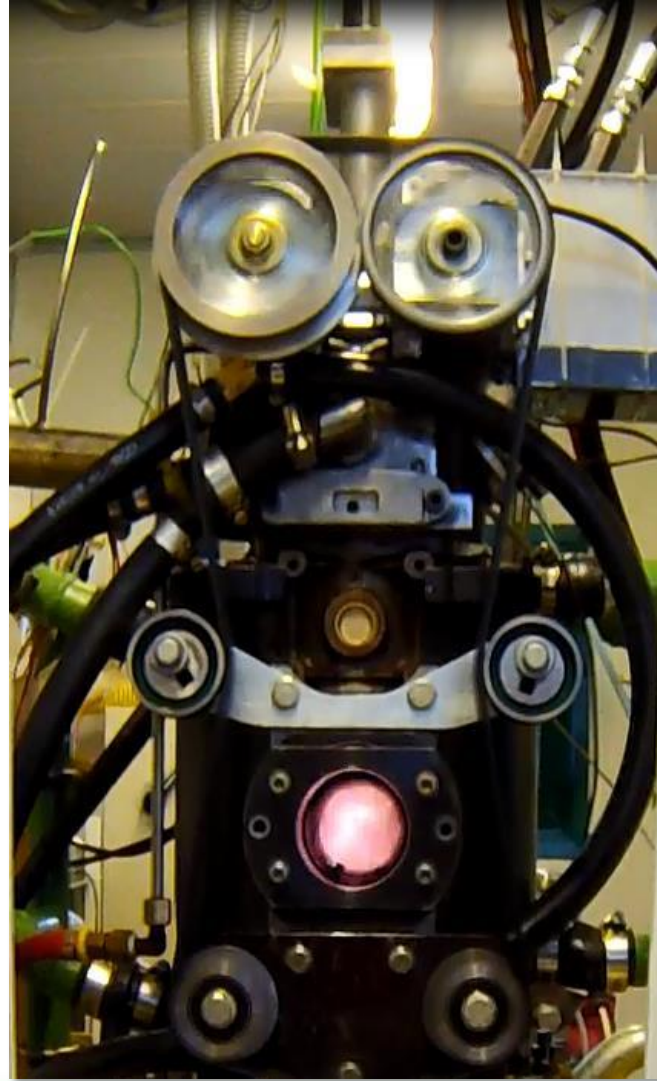
# Optical access SI engine

## Single cylinder optical engine

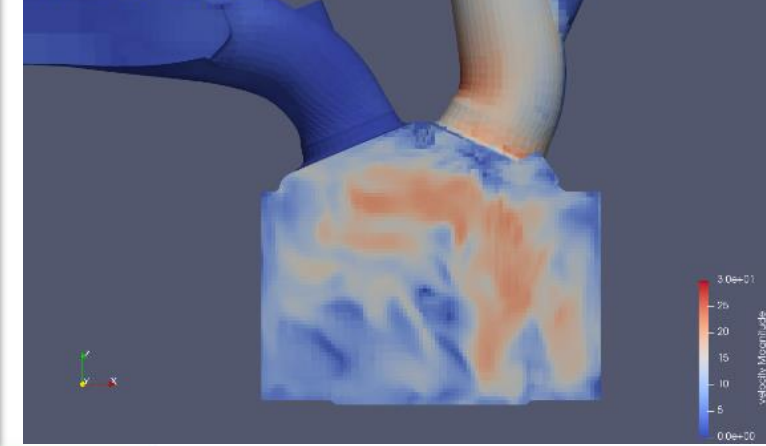
No. of valves	4
Bore	85 mm
Stroke	88 mm
Fueling	PFI (or DI)
CR	9
Chamber type	Pent-roof
Optical access	Bowditch type

## Conditions (low load & speed)

IMEP	~ 5 bar (@ $\lambda=1$ )
Speed	1000 rpm
$\lambda$	1.0 --> lean limit
Spark Advance	Adjusted to MBT
Modes	Fixed throttle, varying injected fuel Fixed fuel, varying air via VVA
Spark Advance	Adjusted to MBT
Fuel	Gasoline, Methane, Hydrogen-Methane blends



Time: 2610.0 CAD



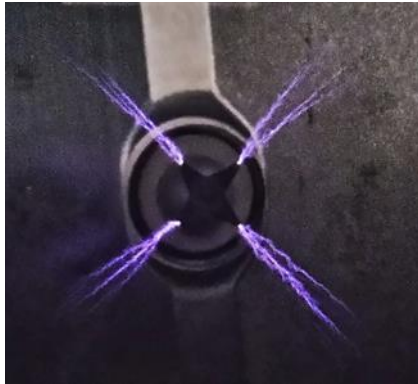
# Ignition systems tested in Perugia University

## Conventional Spark



High temperature plasma

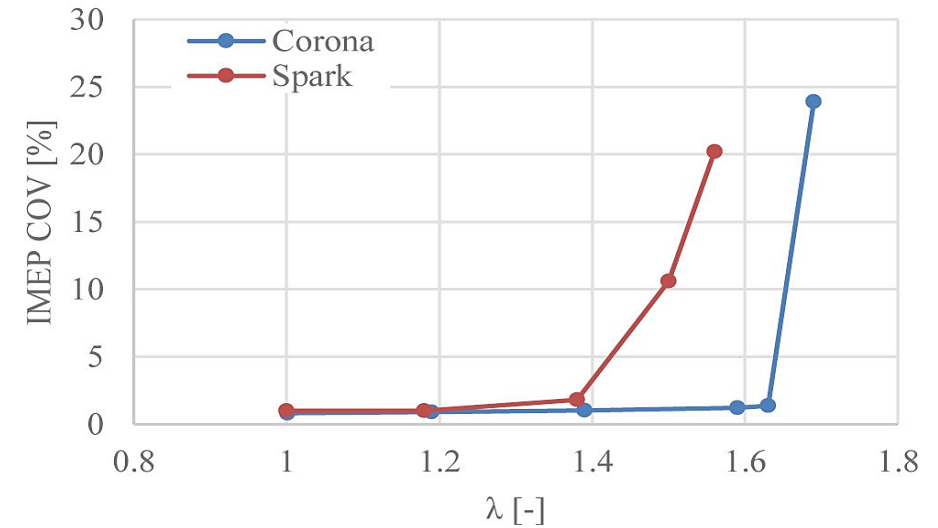
## Advanced Corona Ignition System



Non-equilibrium plasma

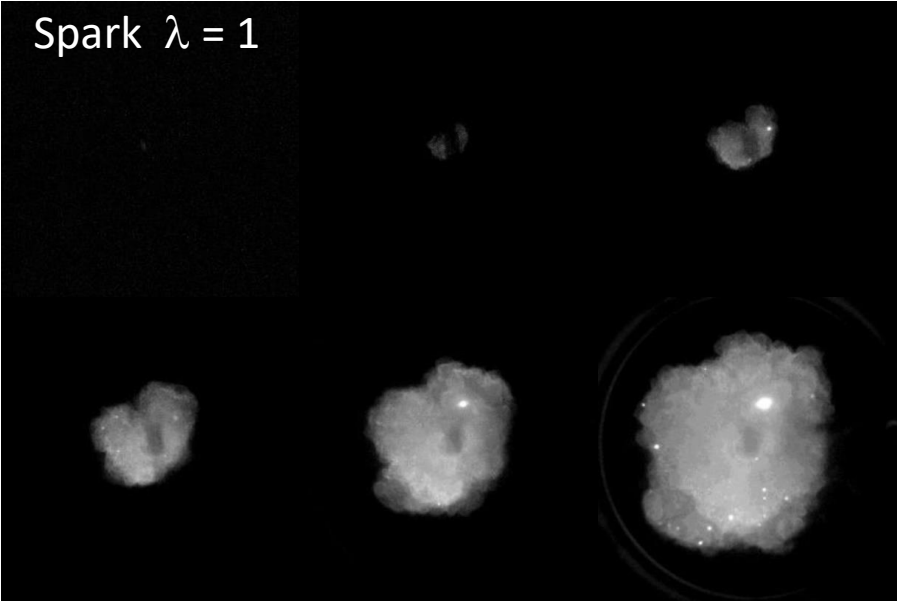


- Extend the lean stable limit
- Improve performance near the knock limit
- Improve EGR tolerance

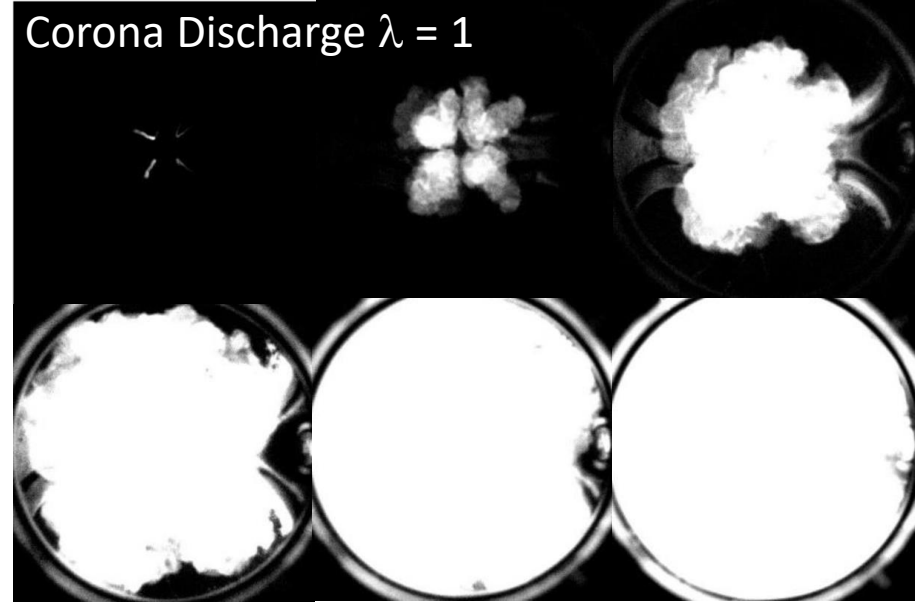


# Spark vs. corona discharge: optical engine flames

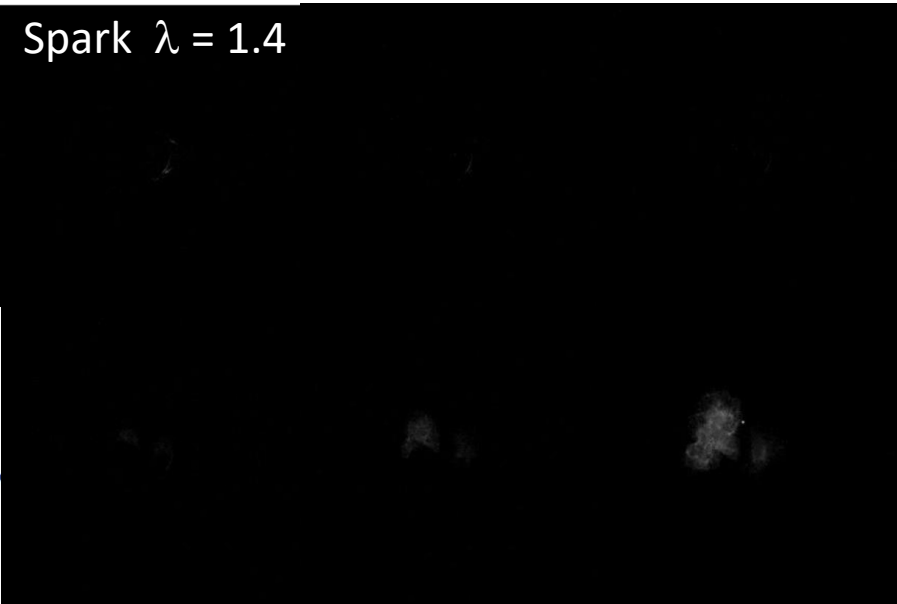
Spark  $\lambda = 1$



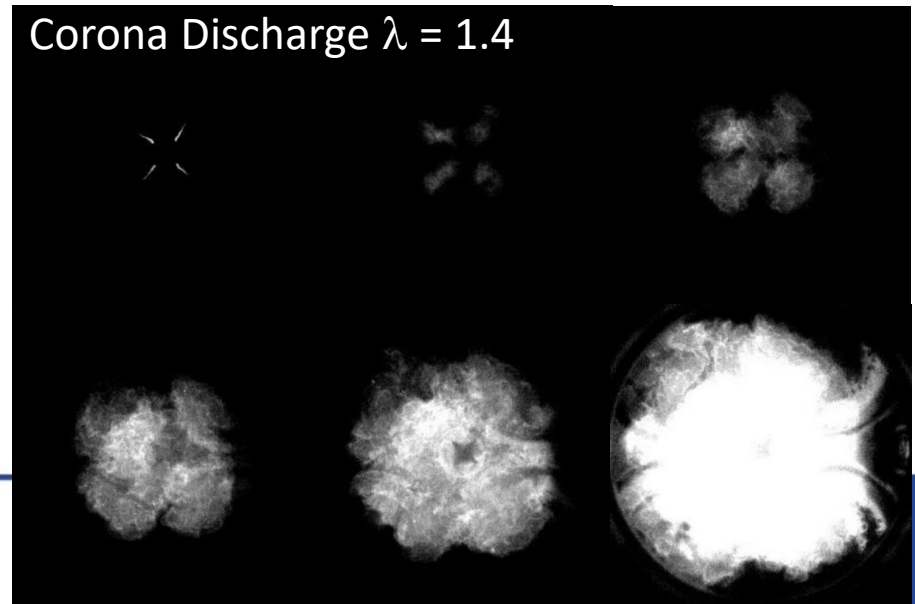
Corona Discharge  $\lambda = 1$



Spark  $\lambda = 1.4$



Corona Discharge  $\lambda = 1.4$



# Outline

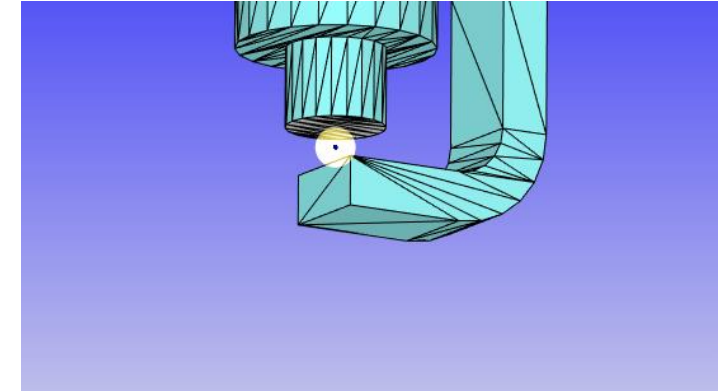
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# CFD Model Setup

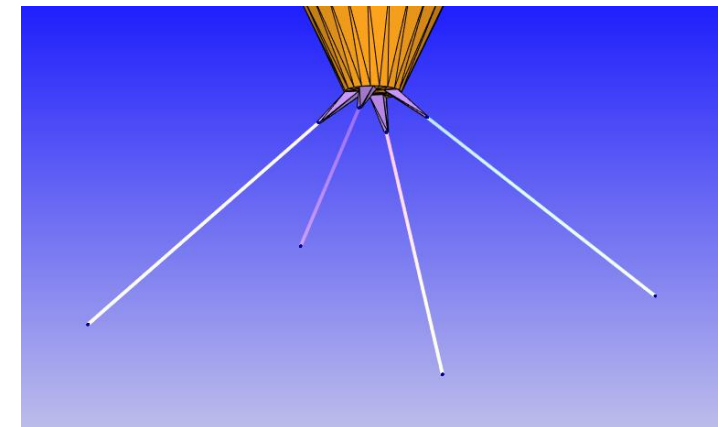
## CFD model in **CONVERGE 3.0**

- Turbulence: **LES** dynamic structure
- Discretization: Space: 2<sup>nd</sup> order, finite volume; Time: 1<sup>st</sup> Euler
- Combustion model:
  - **TFM** coupled with Perfectly Stirred Reactor (**PSR**), SAGE solver and adaptive zoning
  - Mech: **LLNL** reduced mech for low-pressure
  - Fuel: Gasoline **RON 95**
- Spark ignition source:
  - deposition: 10 mJ of energy (breakdown: 5 mJ over 0.5 CAD; arc-glow: 5 mJ over 10 CAD)
  - shape: sphere with 4 mm radius
- Corona ignition source:
  - deposition: 48 mJ of energy over 1.8 CAD (300  $\mu$ s @ 1000 rpm)
  - shape: 4 cylinders with 0.0625 mm radius and 10.7 mm height

Spark



Corona





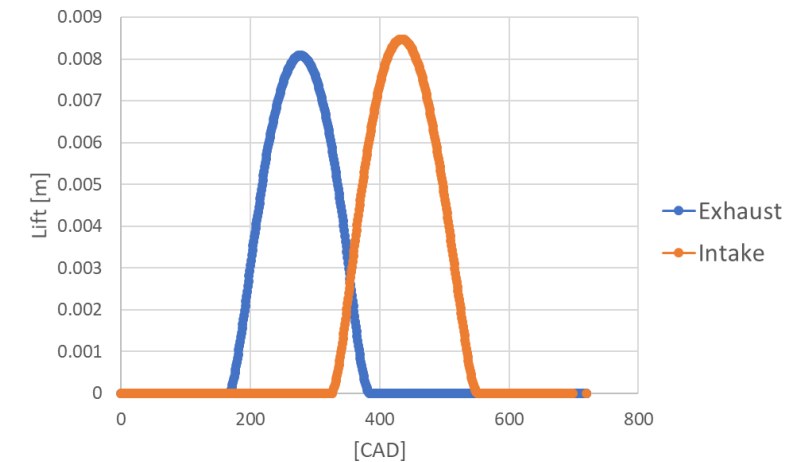
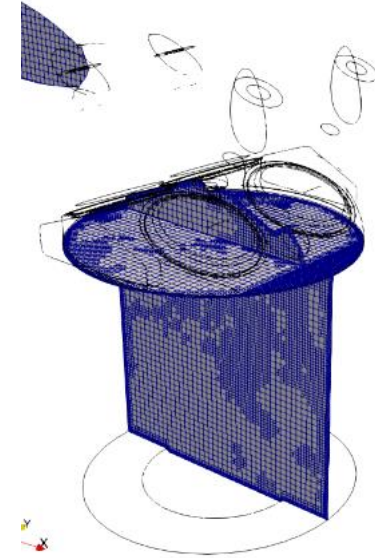
# CFD Model Setup

- Grid:

Base grid size outside the cylinder	8 mm
Base grid size in the cylinder	1 mm
Velocity AMR size (and level)	0.5 mm (4)
TFM - AMR size (and level)	0.25 mm (5)
Minimum grid size (around spark)	0.125 mm

- Boundary conditions:




Engine speed	1000 rpm
$\lambda$	1.0 --> lean limit
Intake lift	IVO = 329 CAD (aTDCf) IVC = 547 CAD (aTDCf)
Exhaust lift	EVO = 170 CAD (aTDCf) EVC = 380 CAD (aTDCf)
Inlet	T = 293 K P = 101325 Pa Premixed $\lambda$
Outlet	T = 800 K P = 101325 Pa



# Outline

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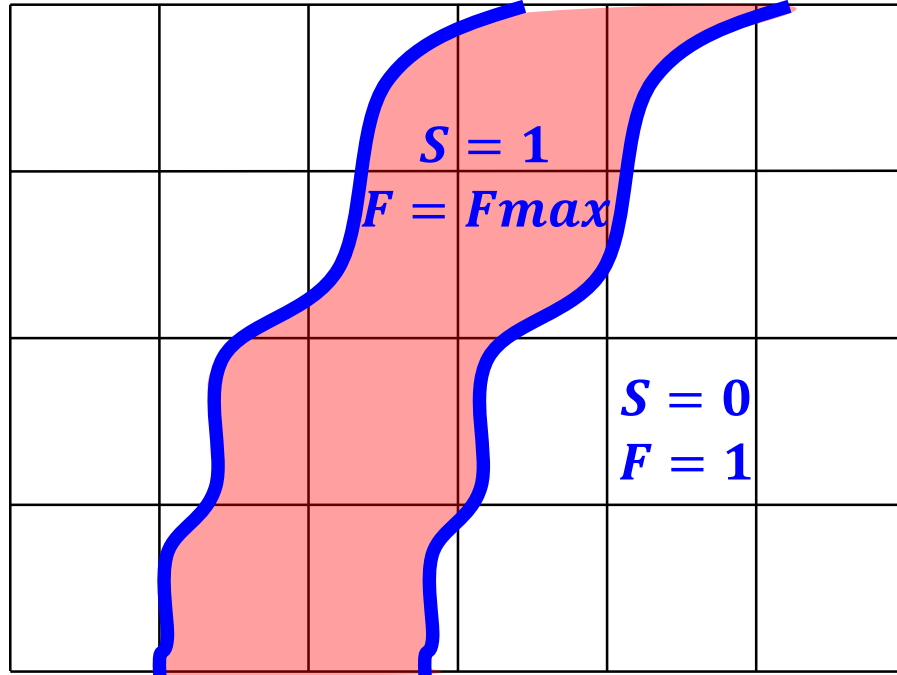
# Why TFM combustion model?

- 1) In LES of premixed flames the cells are not fine enough to resolve the laminar flame thickness  TFM increases the flame thickness without changing the laminar flame-speed  The macroscopic combustion dynamics can be simulated without resolving the flame front explicitly
- 2) TFM is coupled with SAGE detailed chemistry solver  Can take into account Thermal and Kinetic Effect to simulate Corona igniters
- 3) TFM can compensate the absence of TCI effects

## Scaling laws

	Diffusivity	Pre-exponential term	Flamespeed	Flame thickness
Thin flame	$D$	$A$	$s_l^0$	$\delta_l^0$
Thickened flame	$E \cdot F \cdot D$	$E \cdot A / F$	$E \cdot s_l^0$	$F \cdot \delta_l^0$

# TFM formulation: flame sensor



**Two options in CONVERGE:**

1. Standard reaction rate model

2. Jaravel's sensor methodology

→ *Necessary in a detailed chemistry context*

## Dynamic TFM modeling framework

only thicken in the flame front

$$F = 1 + (F_{max} - 1)S$$



*This F is the local thickening factor*

S=0 → F=1 (away from the flame front)

S=1 → F=F<sub>max</sub> (in the flame front)

## Definition of a flame sensor S

$$S = \max \left[ \min \left( \beta \frac{|\dot{\omega}_k|}{|\dot{\omega}_k|_{1D}^{max}} - 1, 1 \right), 0 \right]$$

# TFM formulation: flame sensor

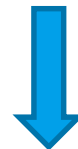
$$S = \max \left[ \min \left( \beta \frac{|\dot{\omega}_k|}{|\dot{\omega}_k|_{1D}^{max}} - 1, 1 \right), 0 \right]$$

- In **1D** table generation, a **steady solver** is used (newton solver)



the reaction rate is directly evaluated from Arrhenius formula, which is independent of time step

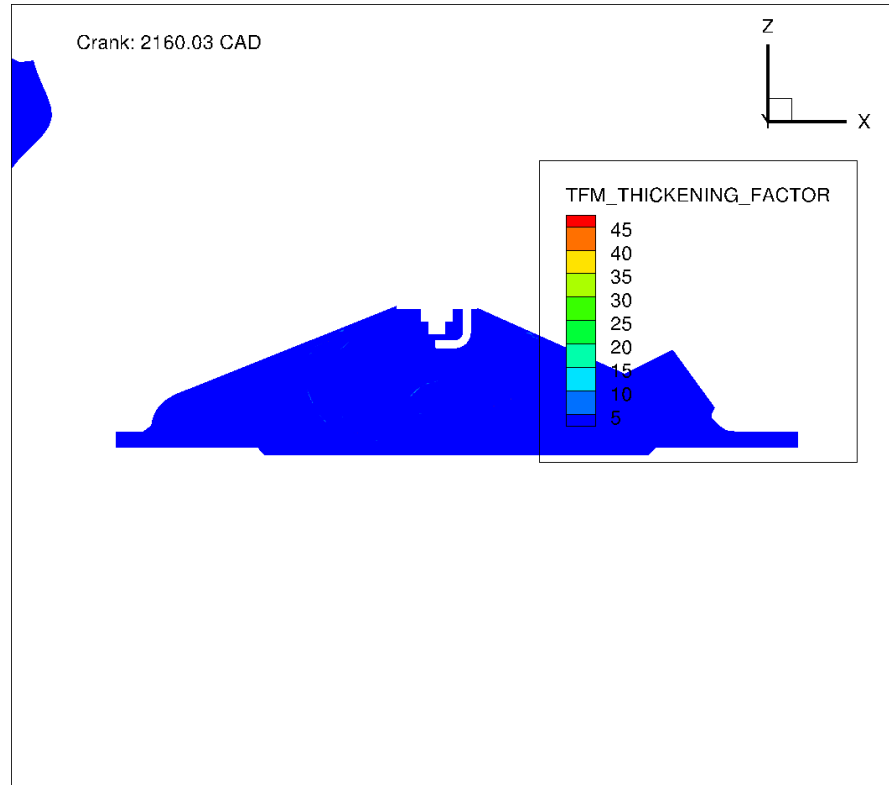
- In **3D** case, the reaction rate is the “averaged” reaction rate between  $t$  and  $t+dt$  and it is **affected by local conditions**



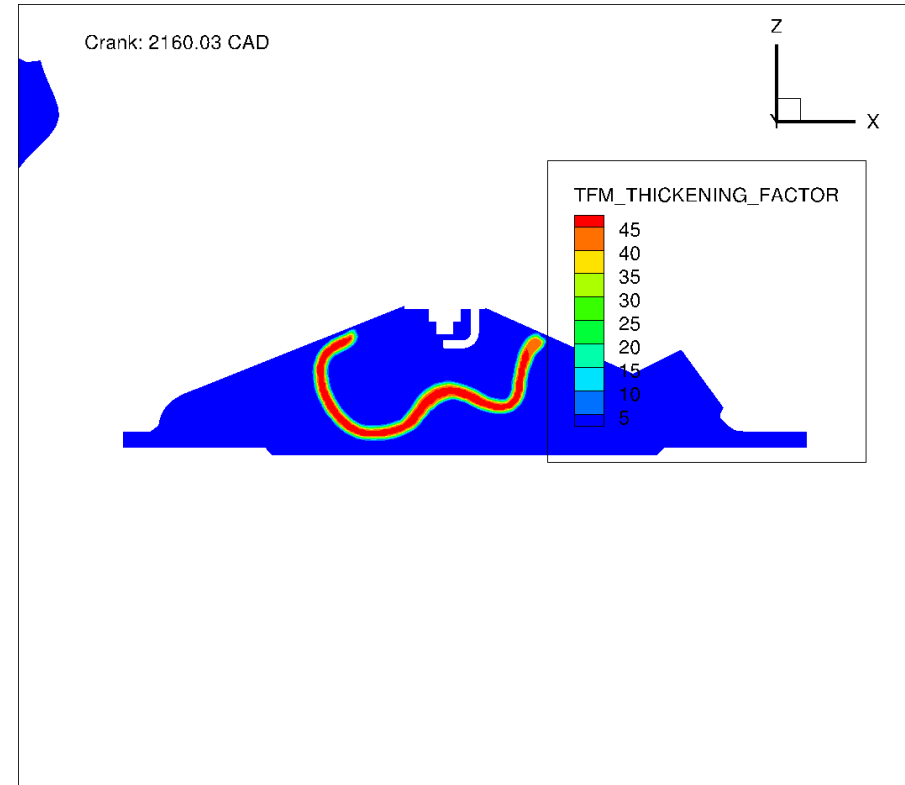
the 3D reaction rate is less than the 1D table value, so the 3D reaction rate is multiplied by the sensor\_slope  $\beta$

# TFM formulation: flame sensor

Sensor slope  $\beta = 10$



Sensor slope  $\beta = 30$



# TFM formulation: thickening options and AMR

## Three options in CONVERGE:

1. Constant maximum thickening factor

$F = \text{constant} \rightarrow n_{\text{res}}$  and  $\delta_F$  are calculated

2. Constant number of grid points across the flame

$n_{\text{res}} = \text{constant} \rightarrow F$  and  $\delta_F$  are calculated

3. Constant thickened flame front and number of grid points across the flame

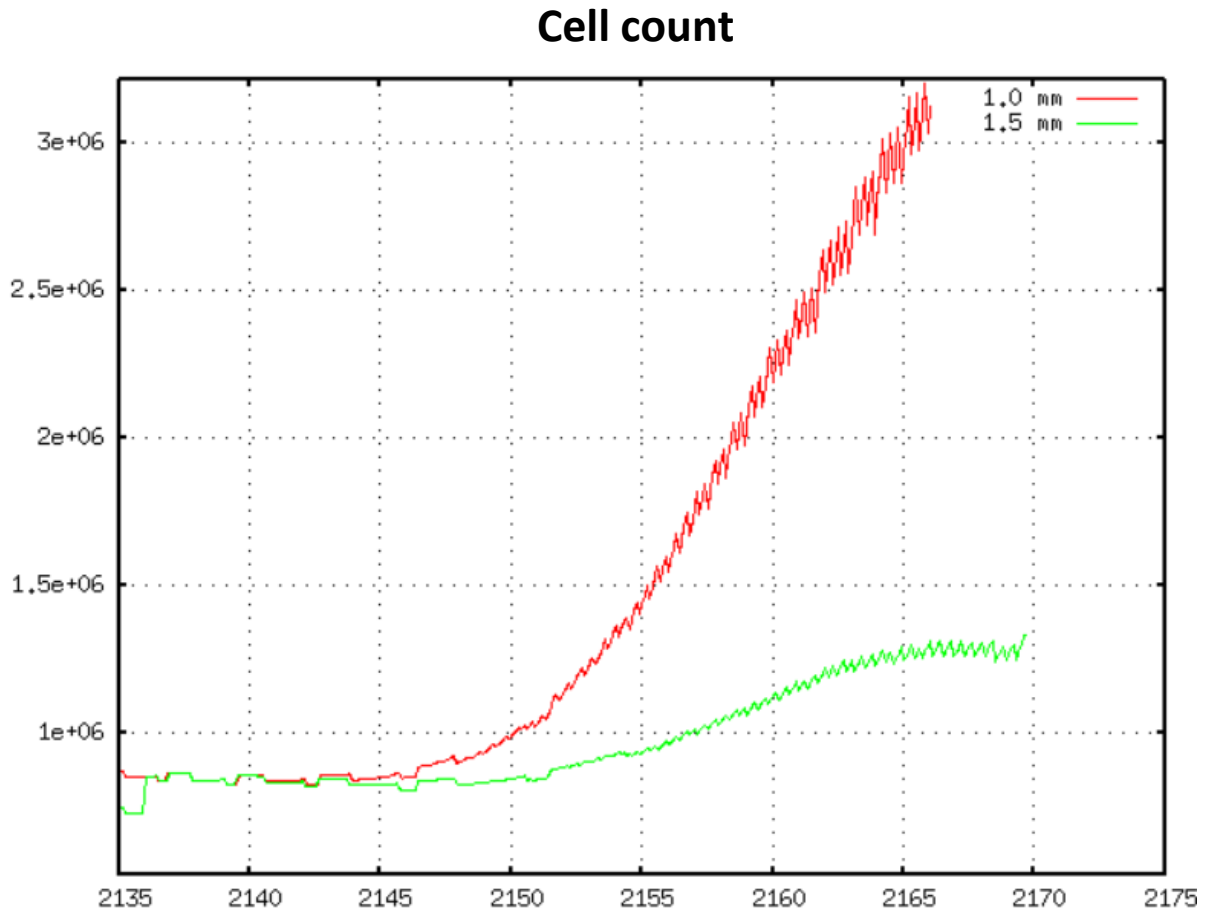
$\delta_F = \text{constant}, n_{\text{res}} = \text{constant} \rightarrow F$  is calculated

$$\delta_F = F * \delta_l^0$$

$$\mathcal{F}_{\text{target}} = \frac{n_{\text{res}} \Delta_x^{\text{AMR}}}{\delta_l^0(\phi)}$$

$$n_{\text{AMR}} = \text{int} \left[ \frac{1}{\log(2)} \log \left( \frac{n_{\text{res}} \Delta_x^{\text{Base}}}{\delta_l^0(\phi) \mathcal{F}_{\text{target}}} \right) \right]$$

# Effect of thickened flame value $\delta_F$



tf\_amr\_thickness\_target  $\delta_F = 1.0$  mm  
and n\_points\_across\_flame = 4



amr\_level = 6  $\rightarrow$  0.125 mm

tf\_amr\_thickness\_target  $\delta_F = 1.5$  mm  
and n\_points\_across\_flame = 4



amr\_level = 5  $\rightarrow$  0.25 mm



# TFM formulation: efficiency function

The efficiency function precursor  $\Xi_{\Delta}$  is introduced to predict the turbulent flame propagation speed:

$$S_T = \Xi_{\Delta} S_l^0$$

**Three options in CONVERGE:**

1. Constant efficiency

2. Charlette's model

$$\Xi_{\Delta} = \left( 1 + \min \left[ \frac{\Delta}{\delta_l^0} - 1, \Gamma_{\Delta} \left( \frac{\Delta}{\delta_l^0}, \frac{u'_{\Delta}}{s_l^0}, \text{Re}_{\Delta} \right) \frac{u'_{\Delta}}{s_l^0} \right] \right)^{\beta}$$

3. Colin's model

$$\Xi_{\Delta} = 1 + \beta_{\text{Colin}} \frac{2 \ln(2)}{3c_{ms} [\text{Re}_l^{1/2} - 1]} \Gamma_{\text{Colin}} \left( \frac{\Delta}{\delta_l^0}, \frac{u'_{\Delta}}{s_l^0} \right) \frac{u'_{\Delta}}{s_l^0}$$

$u'_{\Delta}$  is the sub-grid scale turbulent velocity, and in CONVERGE can be based on curl of the resolved velocity or based on subgrid tke

The efficiency function E is calculated by

$$E = \frac{\Xi|_{\delta=\delta_l^0}}{\Xi|_{\delta=F\delta_l^0}}$$

# Effect of uprime\_multiplier

LLNL mech with RON 95

SA = -23 CAD

TFM start = -20 CAD

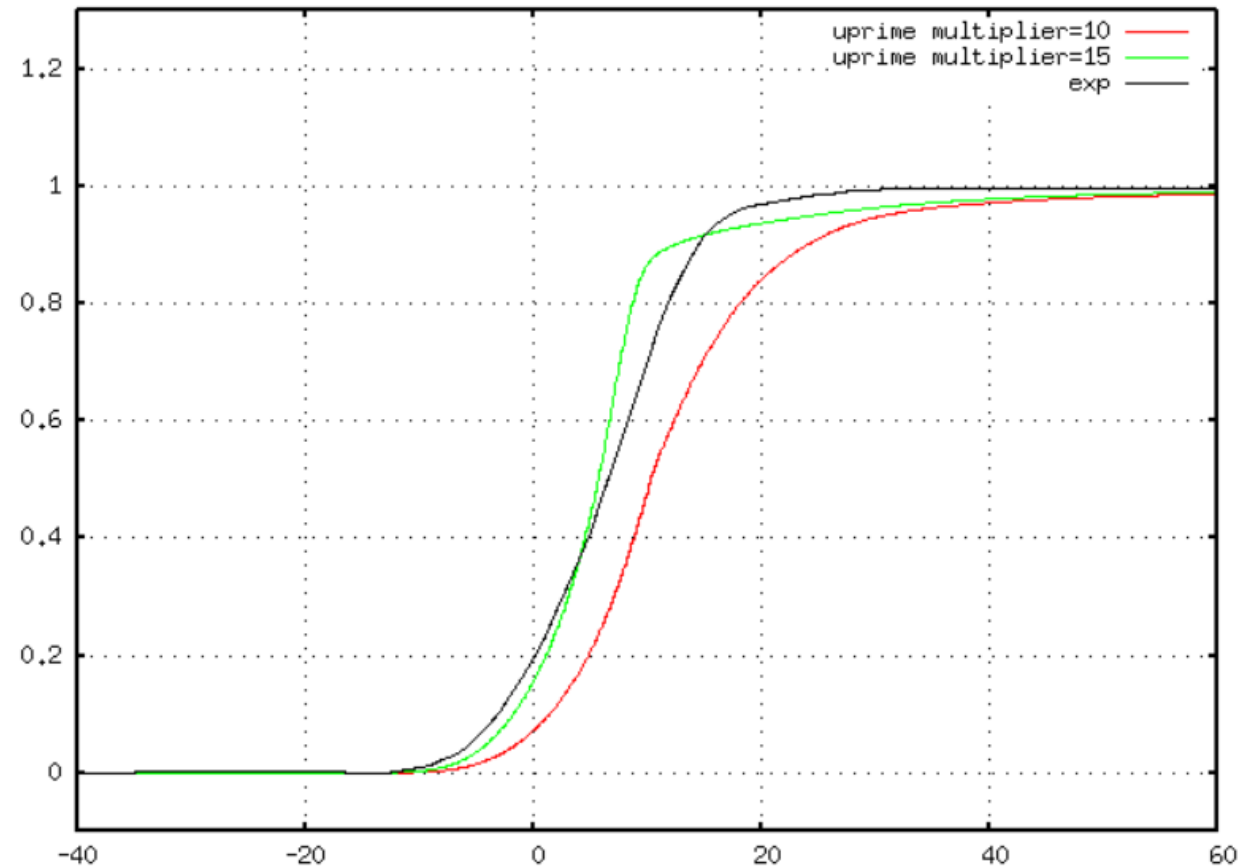
beta\_charlette = 0.65

uprime\_multiplier

10

15

Mass fraction burned



# Effect of Beta\_Charlette

LLNL mech with RON 95

SA = -23 CAD

TFM start = -20 CAD

uprime\_multiplier = 10

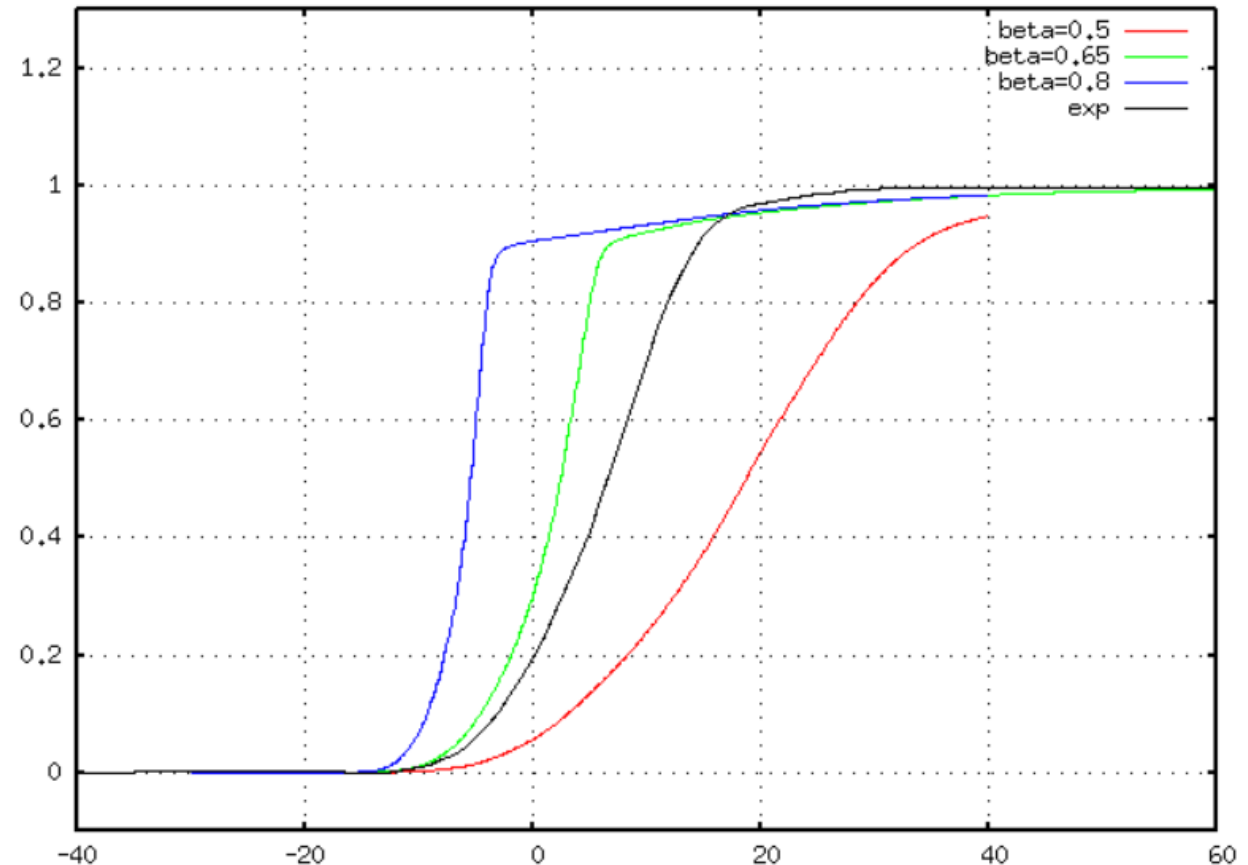
beta\_charlette

0.5

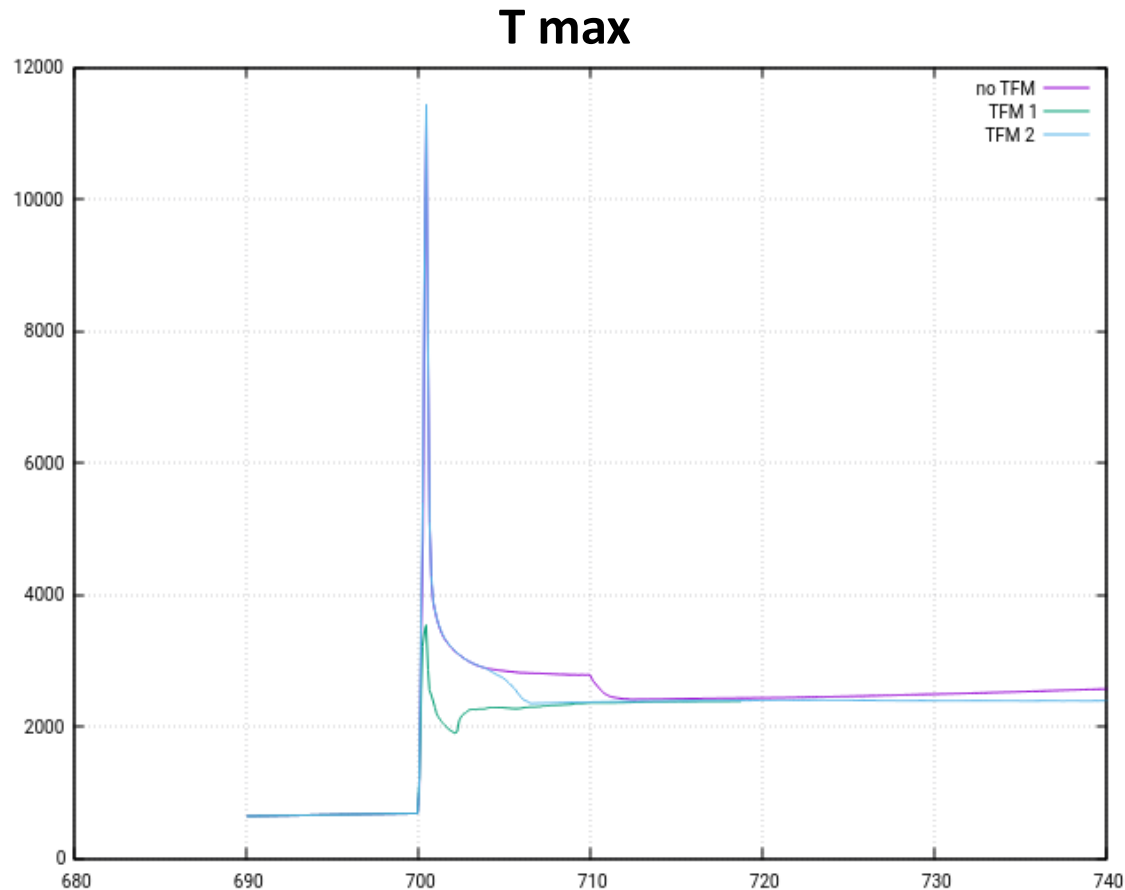
0.65

0.8

Mass fraction burned



# Effect of TFM start timing



SA = -20 CAD





TFM 1: TFM start timing = -20 CAD

TFM 2: TFM start timing = -17 CAD

- Thickened flame procedure affects the ignition, the max temperature decreases because more diffusion is added.
- The thickening procedure should be avoided when the flame kernel is not yet established.

The TFM start timing is set to 3 CAD after the ignition for all cases (manual)

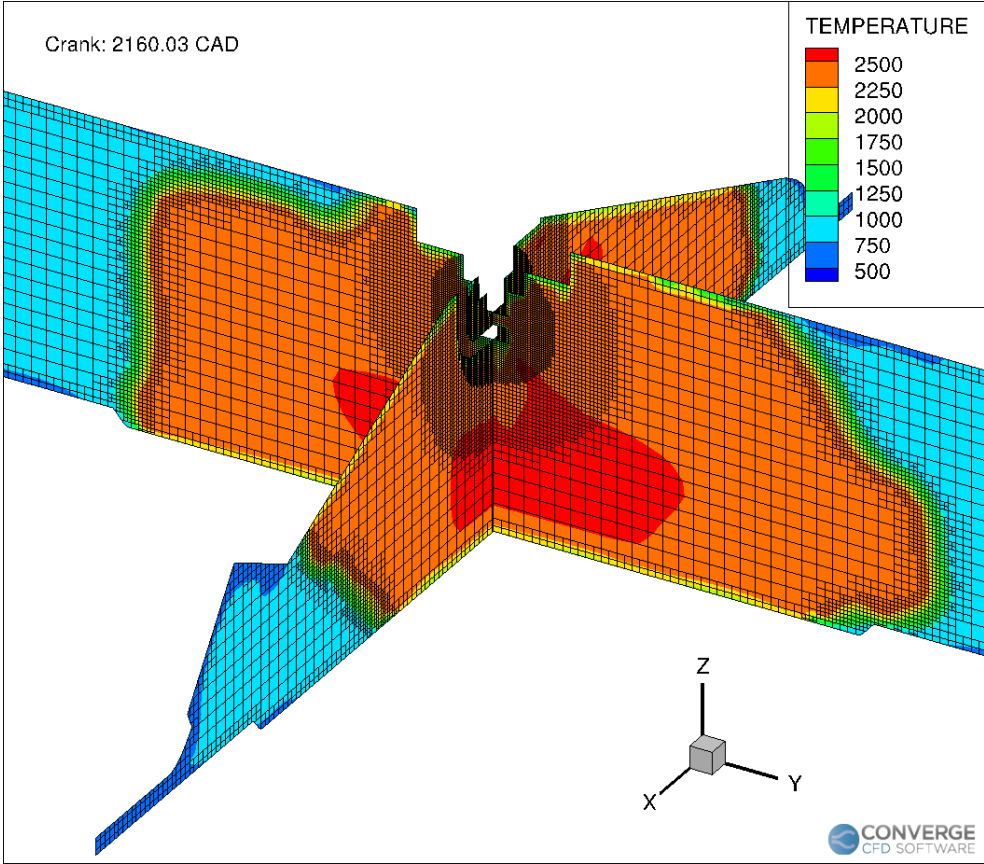
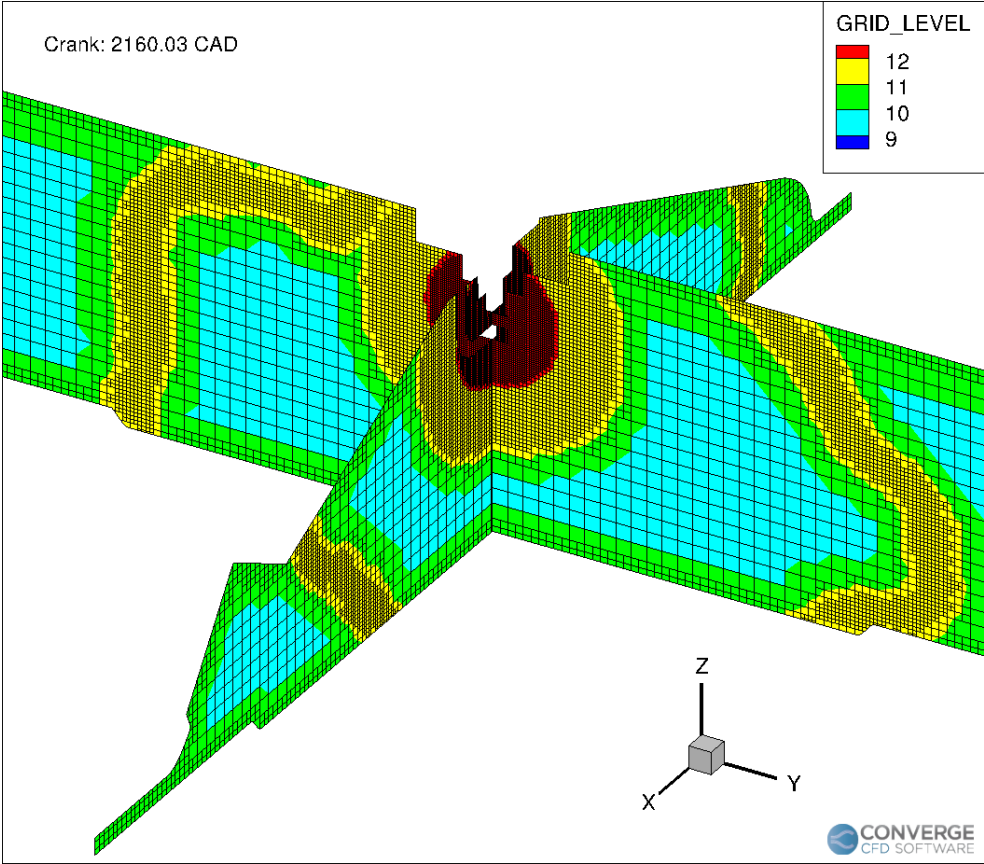
# Summary TFM setup

- TFM flame sensor: Jaravel's sensor methodology  sensor\_slope  $\beta = 30$
- TFM thickening option: Constant thickened flame front and number of grid points across the flame  tf\_amr\_thickness\_target  
 $\delta_F = 1.5$  mm  
n\_pts\_across\_flame = 4  flame resolution = 0.25 mm  
(amr\_level = 5)
- TFM efficiency function: Charlette's model  uprime\_multiplier = 10  
beta\_charlette = 0.6
- TFM start timing: manually set to 3 CAD after the ignition, for all cases

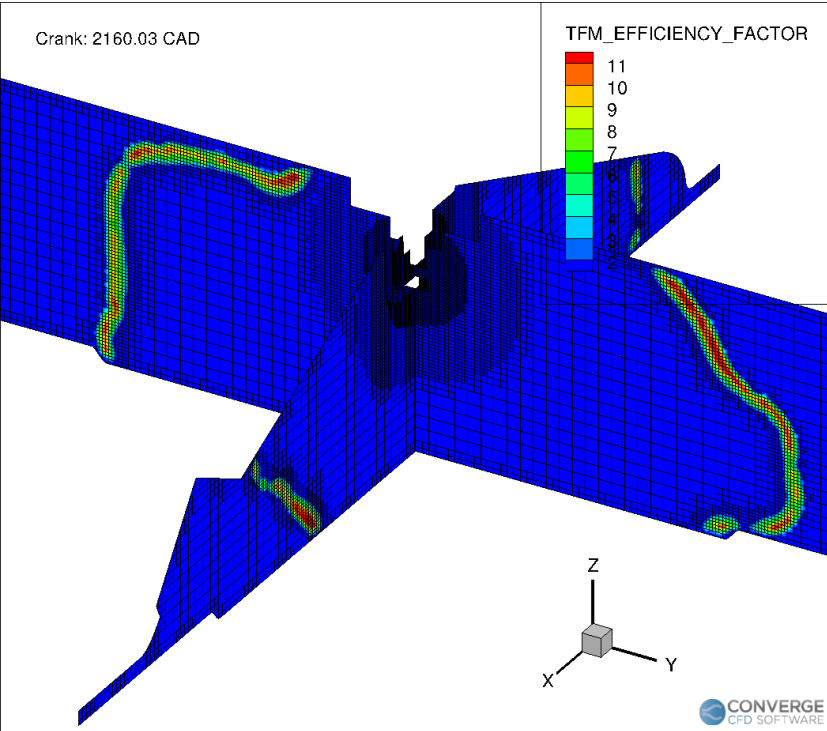
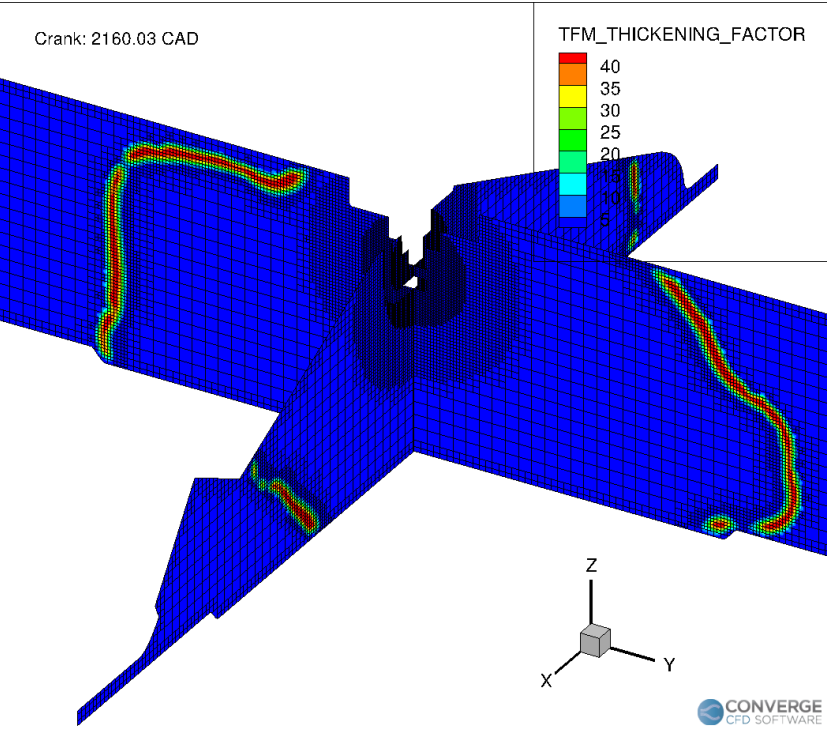
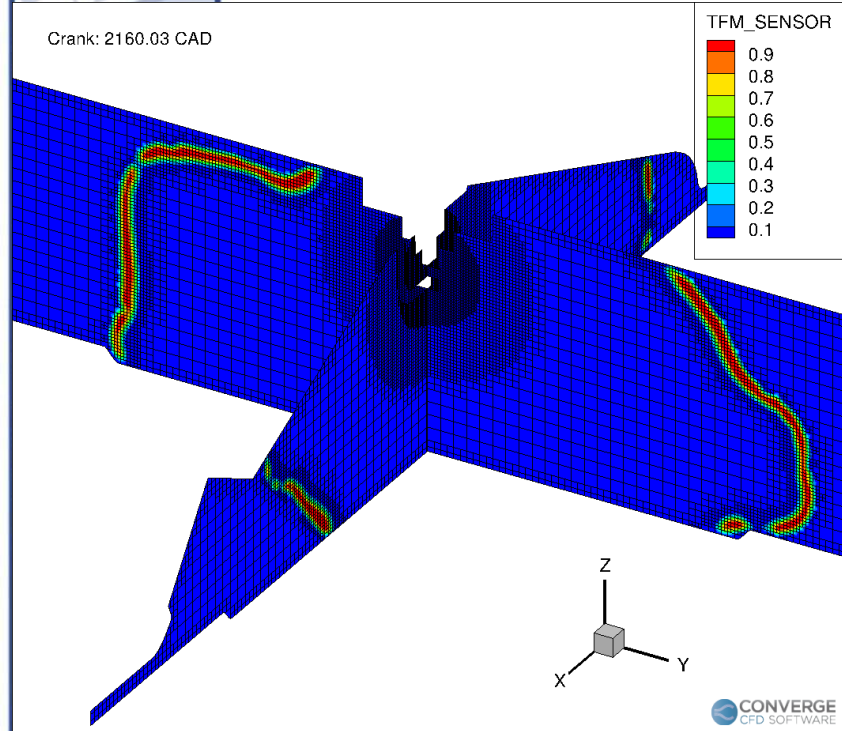
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# TFM 3D output

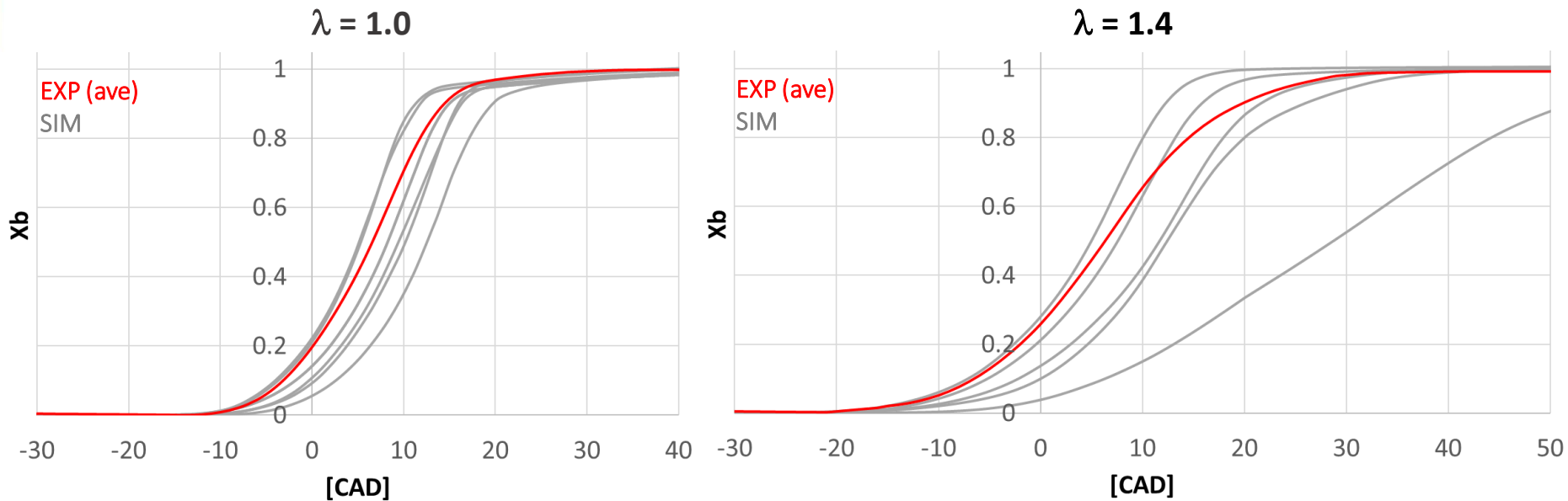


# TFM 3D output





# Mass fraction burned at different $\lambda$ – Spark



- IT\_exp: 20 CAD bTDCf
- TFM\_start: 20 CAD bTDCf
- IT\_num: 23 CAD bTDCf

- IT\_exp: 40 CAD bTDCf
- TFM\_start: 40 CAD bTDCf
- IT\_num: 43 CAD bTDCf

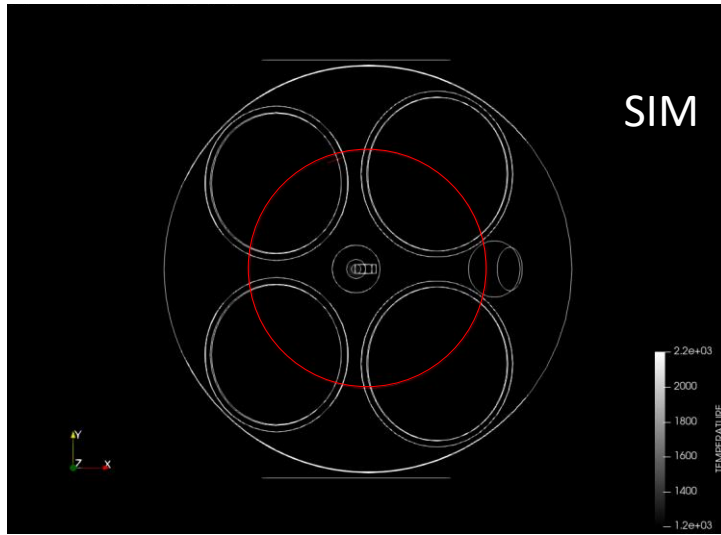
## CASE SETUP

Fuel: Gasoline RON95  
Sensor slope: 30  
Uprime\_multiplier: 10  
Beta\_Charlette: 0.6  
Spark energy: 5+5 mJ

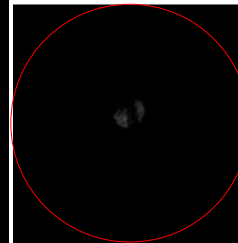
- Combustion rates are satisfactorily predicted

# Flame imaging comparison – Spark $\lambda=1.0$

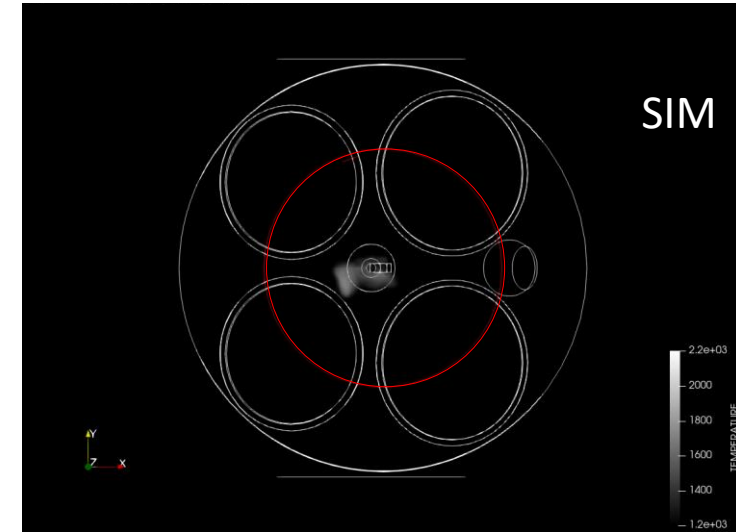
Timing  
3 CAD  
aIT



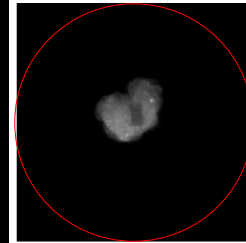
EXP



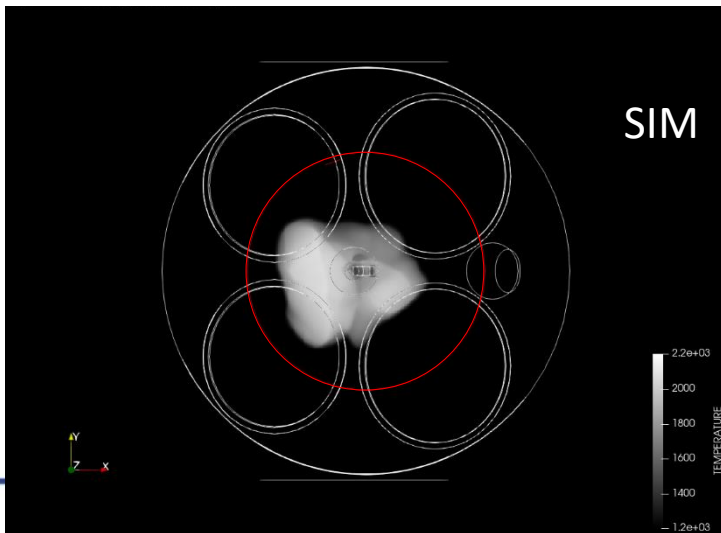
Timing  
9 CAD  
aIT



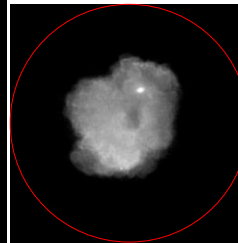
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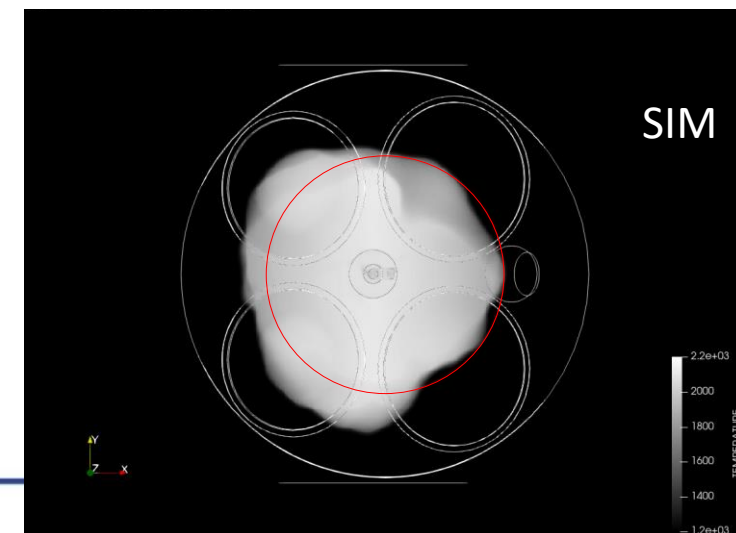
Timing  
15 CAD  
aIT



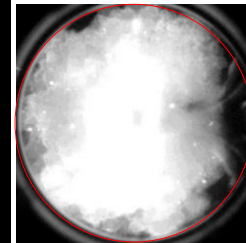
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Timing  
23 CAD  
aIT

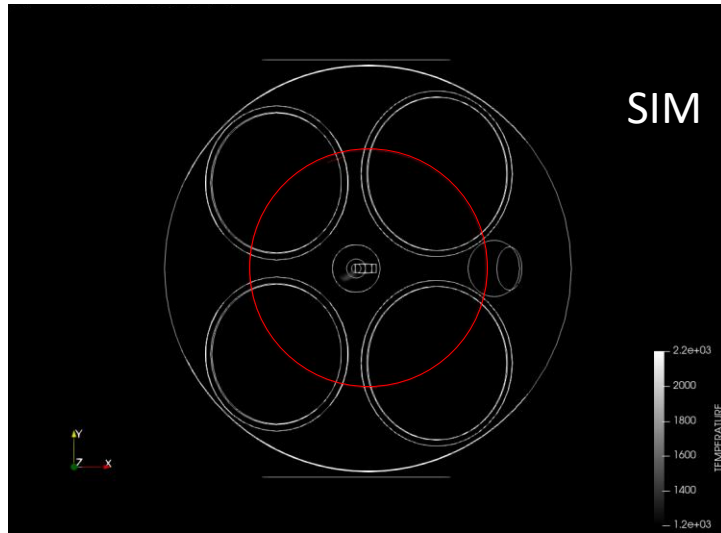


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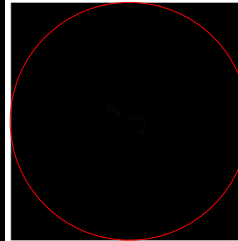


# Flame imaging comparison – Spark $\lambda=1.4$

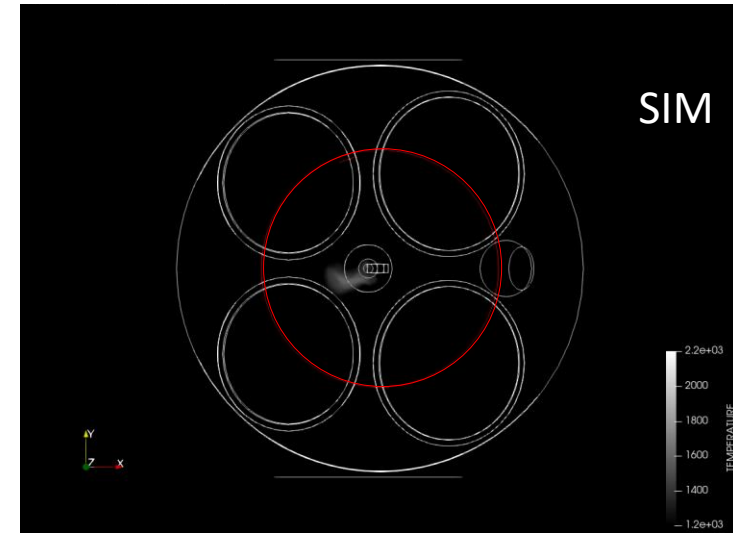
Timing  
9 CAD  
aIT



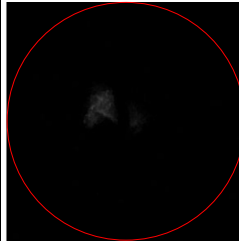
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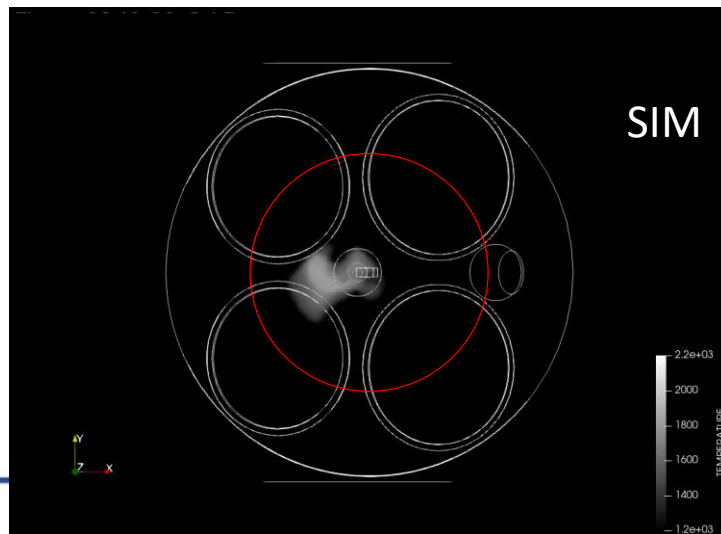
Timing  
19 CAD  
aIT



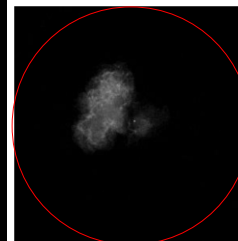
EXP



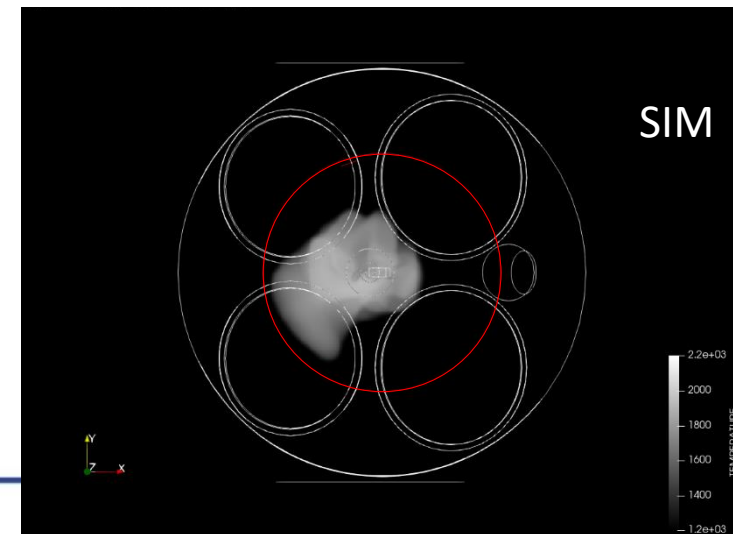
Timing  
25 CAD  
aIT



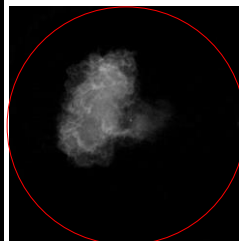
EXP



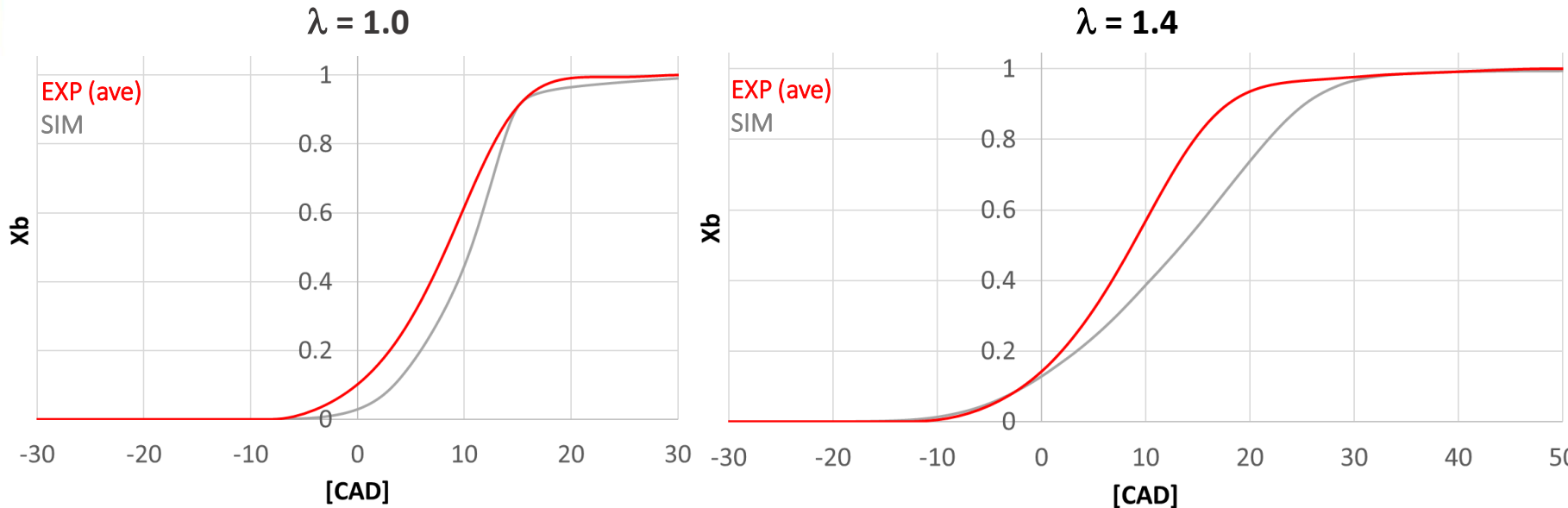
Timing  
31 CAD  
aIT



EXP



# Mass fraction burned at different $\lambda$ – ACIS



- IT\_exp: 6 CAD bTDCf
- TFM\_start: 9 CAD bTDCf
- IT\_num: 6 CAD bTDCf

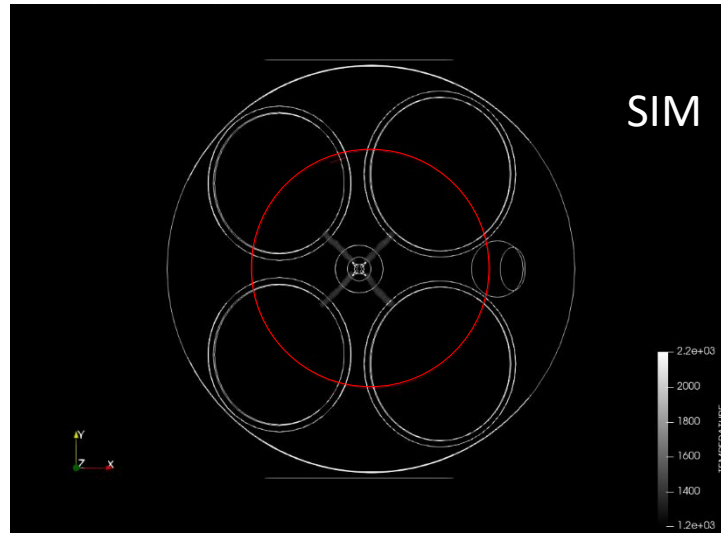
- IT\_exp: 16 CAD bTDCf
- TFM\_start: 19 CAD bTDCf
- IT\_num: 16 CAD bTDCf

## CASE SETUP

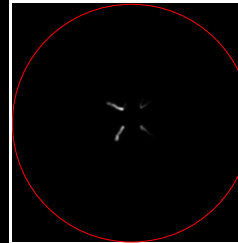
Fuel: Gasoline RON95  
Sensor slope: 30  
Uprime\_multiplier: 10  
Beta\_Charlette: 0.6  
Deposition: 48 mJ over  
1.8 CAD (300  $\mu$ s @ 1000  
rpm)

# Flame imaging comparison – ACIS $\lambda=1.0$

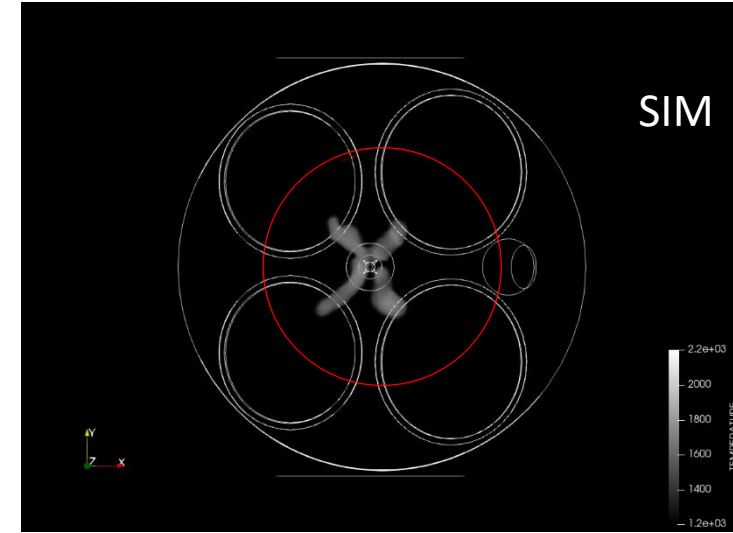
Timing  
1 CAD  
aIT



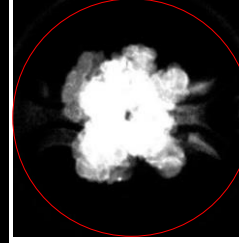
EXP



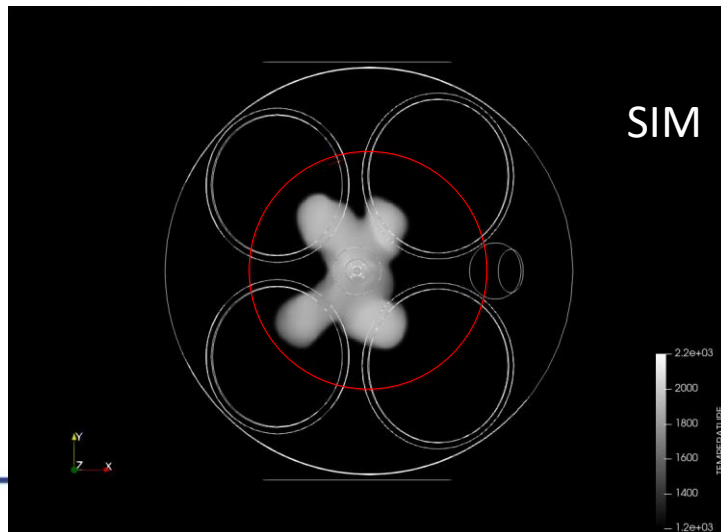
Timing  
5 CAD  
aIT



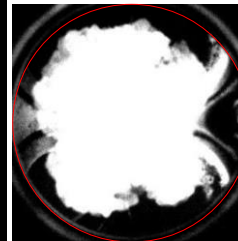
EXP



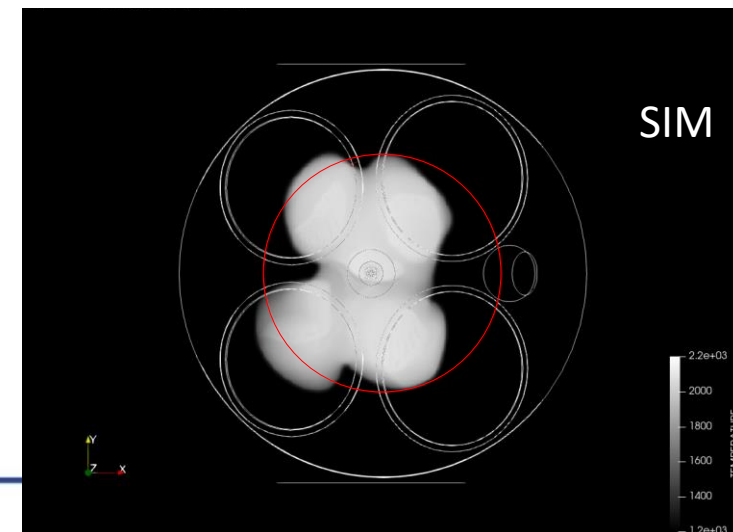
Timing  
9 CAD  
aIT



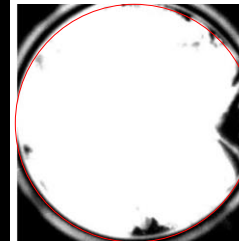
EXP



Timing  
13 CAD  
aIT

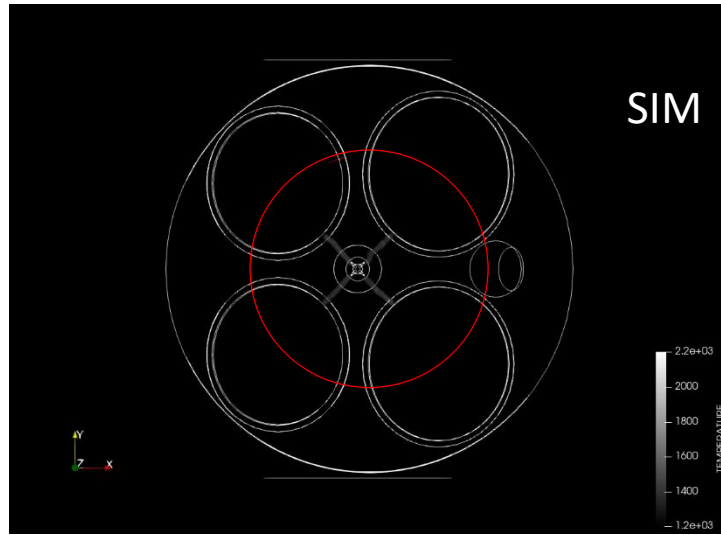


EXP



# Flame imaging comparison – ACIS $\lambda=1.4$

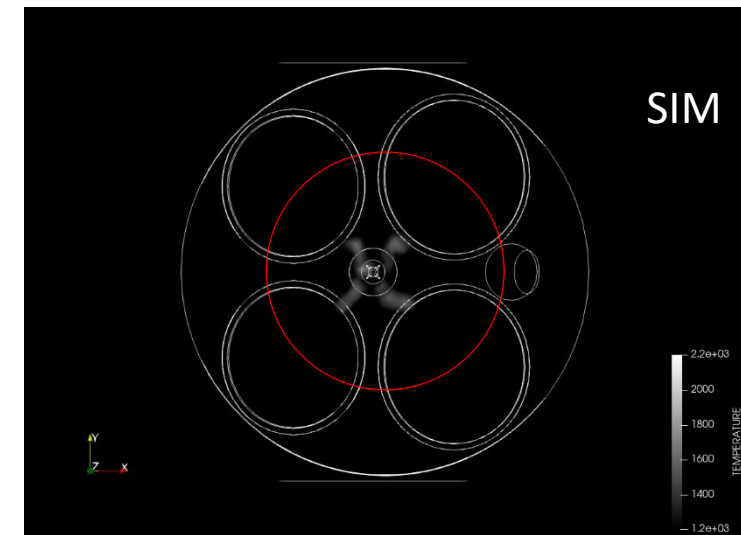
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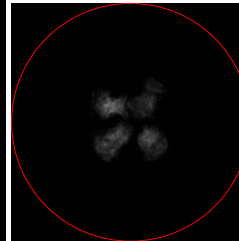
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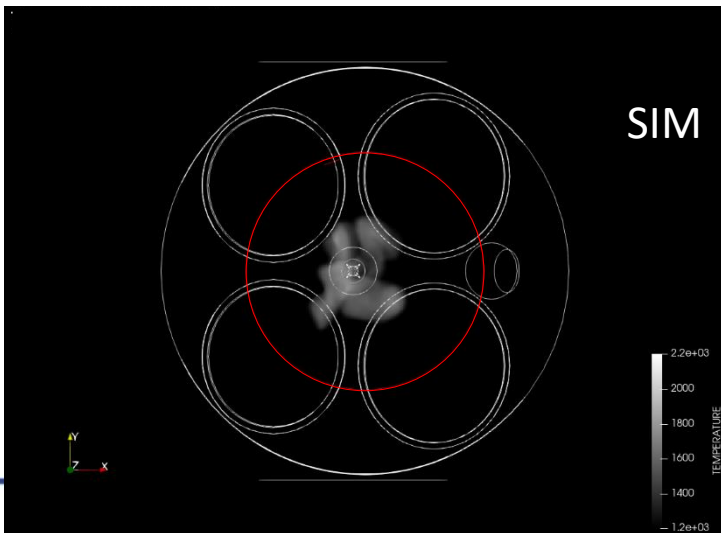
Timing  
5 CAD  
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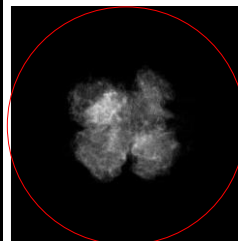
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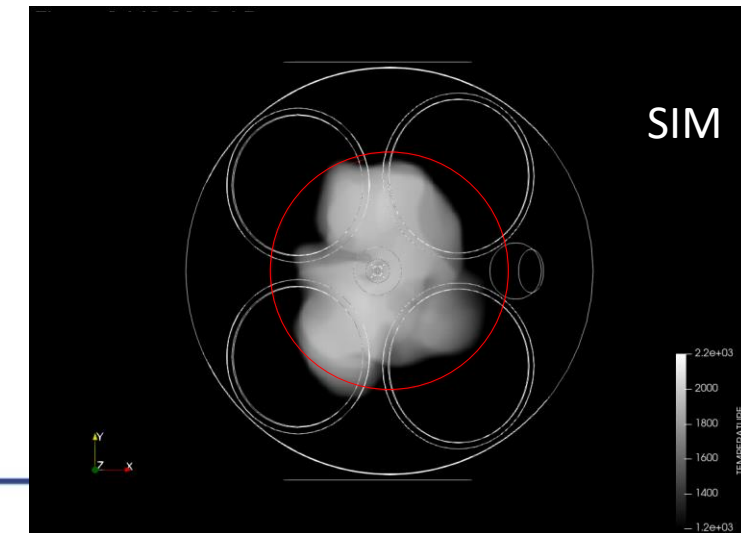
Timing  
9 CAD  
aIT



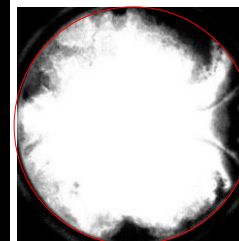
EXP



Timing  
19 CAD  
aIT



EXP



# Outline

1. Experimental Setup
  - Optical access SI engine
  - Ignition systems tested in Perugia University
2. CFD Model Setup
3. TFM combustion model
  - Why TFM?
  - Flame sensor
  - Thickening options and AMR
  - Efficiency function
  - Effect of the calibration parameters
4. Cycle to cycle variability prediction
  - Multicycle LES simulations at different conditions
  - Mass fraction burned at different  $\lambda$
  - Flame comparison at different  $\lambda$
5. Conclusions and next steps

# Conclusions

- The TFM combustion model is explored in detail
- A good setup has been defined
- Global (xb) and local (flame image) results are in good agreement with experimental data

## Next Steps

- A sub-model to manage the transition and activation of the TFM is necessary
- The dynamic beta Charlette formulation could be implemented
- More cycles are needed to better understand the statistics and analyze the CCV





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