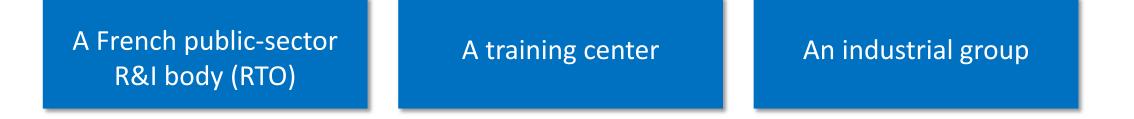


# PISTON ENGINE COMBUSTION WITH ECFM3Z: KEY ELEMENTS OF IFPEN COMBUSTION MODELING APPROACH

**Olivier Colin (IFPEN),** Stéphane Chevillard (IFPEN), Julien Bohbot (IFPEN), Anthony Velghe (IFPEN), Mingjie Wang (CSI)



#### **IDENTITY CARD OF IFPEN**



An international scope in the fields of energy, transport and the environment



### **IDENTITY CARD OF IFPEN**

#### SUSTAINABLE MOBILITY

1,660 people

of whom



155 doctoral and post-

doctoral researchers



**2** sites: Rueil (near Paris) and Solaize (near Lyon)



1,130 researchers



A very high-quality technical environment: testing resources, equipment, **110** teraflop supercomputer

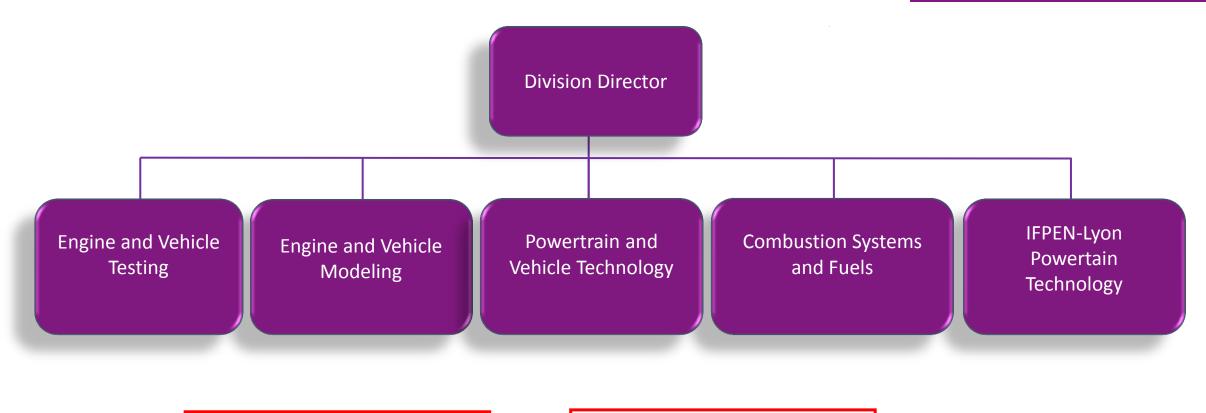


More than **50** professions, from geological engineers to powertrain engineers





#### POWERTRAIN AND VEHICLE DIVISION



96 Engineers 63 Technicians 18 PhD students 2 Post-docs 2 Apprentices 11 Engine test benchs 5 Optical test benchs



# OUTLOOK OF THE PRESENTATION

The ECFM3Z combustion model

Diesel application

• SI application

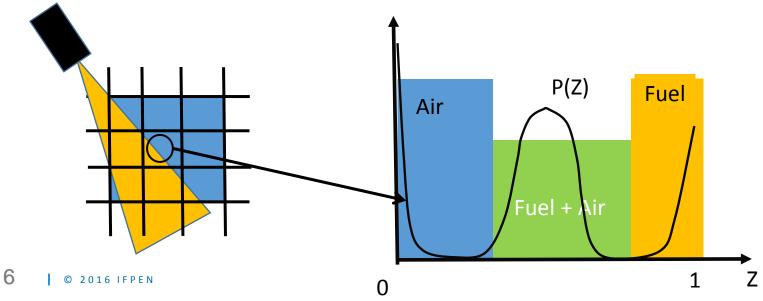
• Future developments in Converge





### THE ECFM3Z COMBUSTION MODEL [1]

- General purpose model developed at IFPEN the last 20 years
  - Based on premixed flame propagation model (ECFM) [2,3] for gasoline engines
  - Spark plug ignition description: AKTIM [4] then ISSIM [5]
  - Knock/auto-ignition model: TKI [6]
  - Local fuel/air ratio fluctuations for Diesel combustion: three mixture fraction description
    - Pure air + EGR
    - Pure gaseous fuel (from evaporating liquid spray)
    - Mixed zone air+EGR+fuel

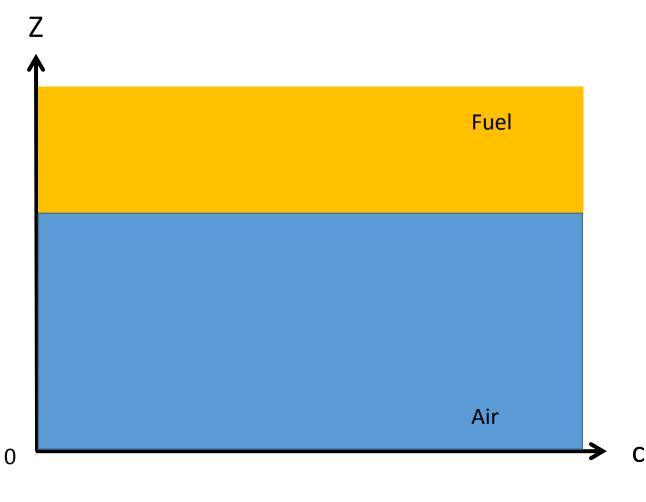


[1] Colin et al, OGST, 2003
 [2] Duclos et al, SAE, 1996
 [3] Colin et al, OGST, 2004
 [4] Duclos et al., COMODIA, 2000
 [5] Colin and Truffin, PCI, 2010
 [6] Colin et al, PCI, 2004



• Fuel and Air initially not premixed

Progress of reaction c = 0

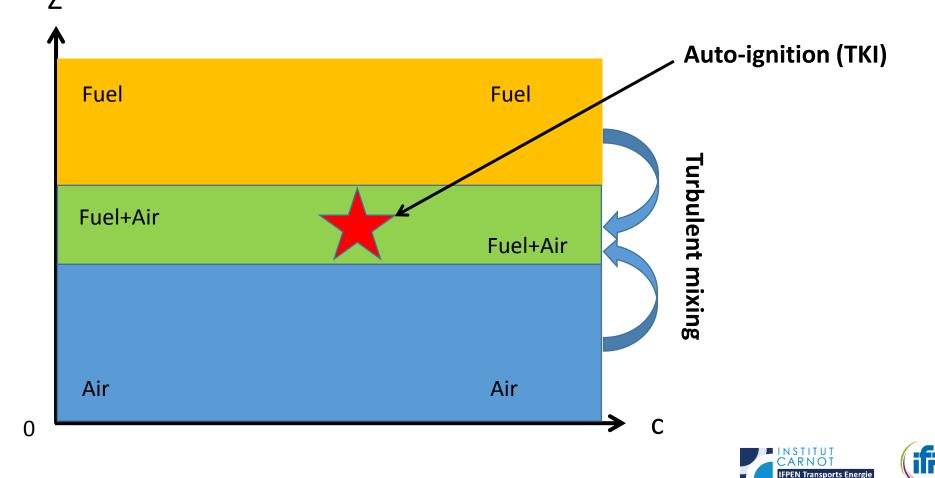


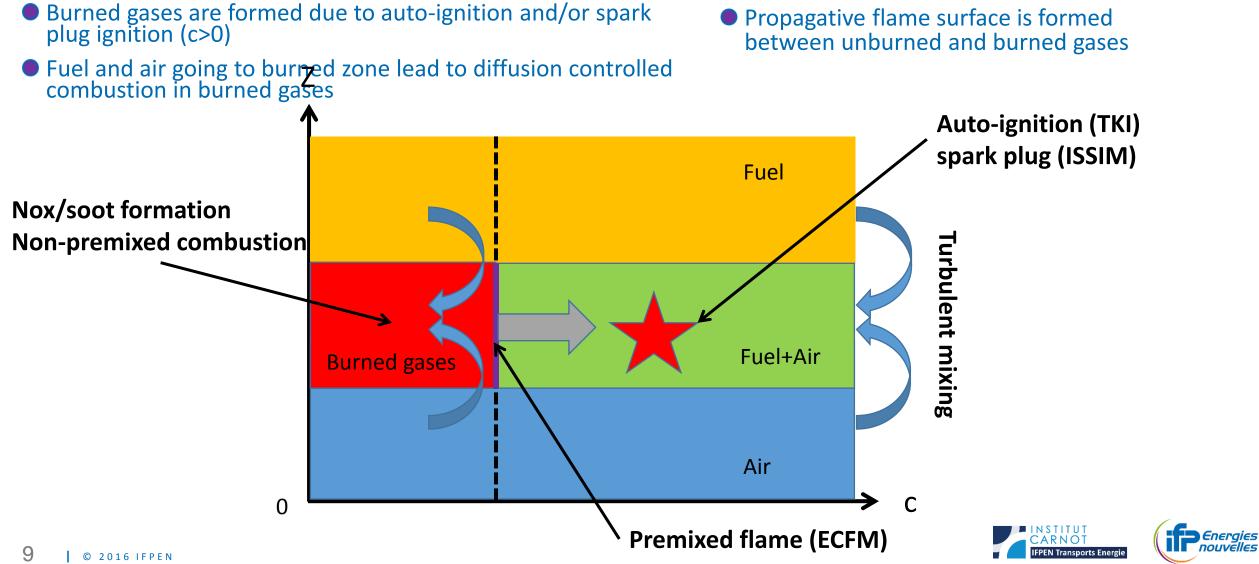
Energies nouvelles

**Transports Energi** 

Energies nouvelles

- Mixed zone is formed
- Auto-ignition description starts in mixed zone
- Progress of reaction is still zero (c = 0)

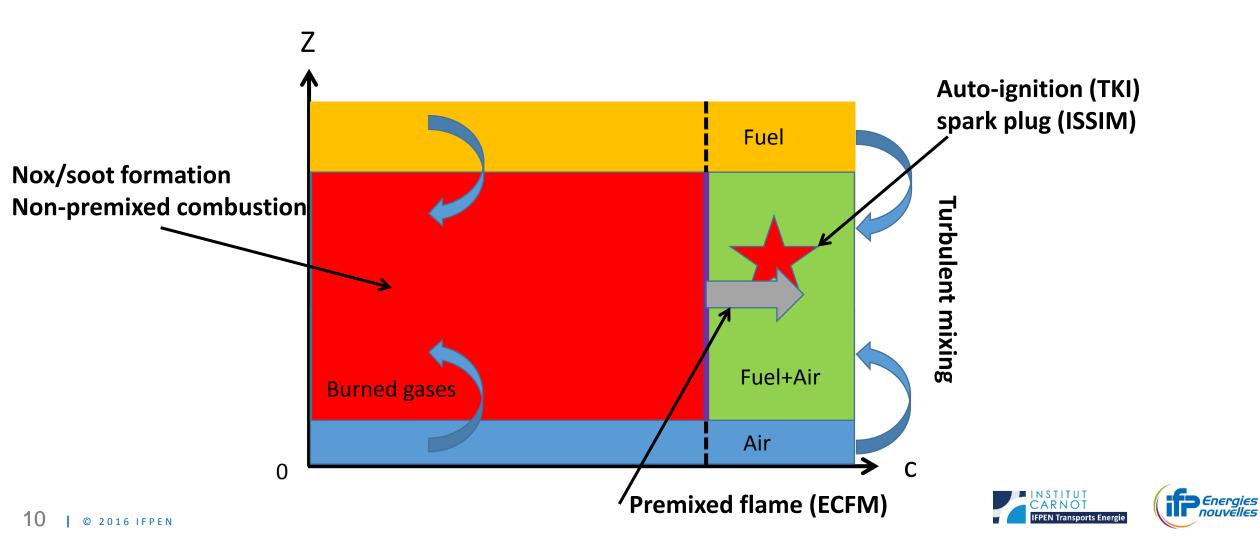




- Mixed zone keeps growing

#### NOx and soot start to form in burned gases

#### Combustion proceeds till c=1 and unmixed zones are void

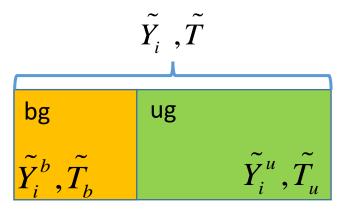


# ECFM3Z UNBURNED/BURNED GASES STATES

• Standard transport equations for species mass fractions Yi and sensible energy

$$\frac{\partial \rho \tilde{Y}_i}{\partial t} + \nabla .(\rho \tilde{u} \tilde{Y}_i) = \nabla .(\mu_t \nabla \tilde{Y}_i) + \rho \tilde{\omega}_i$$
 Chemical source term contributions (ECFM+TKI+ISSIM+post-oxidation)

- Same equations for species and energy passives
- Local fresh gases composition (i=O<sub>2</sub>, Fuel, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>) and temperature (Tu) can be deduced
- Local burned gases composition and temperature (Tb) can be deduced





# ECFM3Z AUTO-IGNITION PROGRESS VARIABLE

 Global progress variable = burned gases fraction in mixed zone=> defined as the ratio of unburned fuel and fuel tracer

 $\tilde{c} = \frac{m_b}{m_u + m_b} = 1 - \frac{\tilde{Y}_F}{\tilde{Y}_{TF}}$ 

• Specific progress of reaction for auto-ignition model (TKI model)

• Fuel burned by auto-ignition 
$$\widetilde{Y}_{F}^{ai}$$
 is given by its transport equation

$$\frac{\partial \bar{\rho} \tilde{Y}_{F}^{ai}}{\partial t} + \nabla .(\bar{\rho} \tilde{u} \tilde{Y}_{F}^{ai}) = \nabla .(\mu_{t} \nabla \tilde{Y}_{F}^{ai}) + \tilde{\phi} \tilde{\psi}_{\tilde{Y}_{F}^{ai}} \leftarrow Chemical source term contribution (TKI)$$



bg ug  $\widetilde{c}$ 



SUSTAINABLE MOBILITY

 $\tilde{c}_{ai} = 1 - \frac{\tilde{Y}_{F}^{ai}}{\tilde{Y}_{TF}}$ 

# LINK BETWEEN ALL PROGRESS VARIABLES

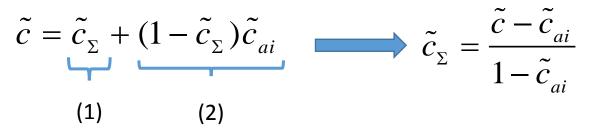
 Premixed flame separates fresh auto-igniting gases and burned gases

 $\tilde{\Phi} = (1 - \tilde{c}_{\Sigma}) \Phi \Big|^{ai} + \tilde{c}_{\Sigma} \Phi \Big|^{b}$ 

 Fresh auto-igniting gases are treated in a bimodal way for simplicity (homogeneous zone in reality)

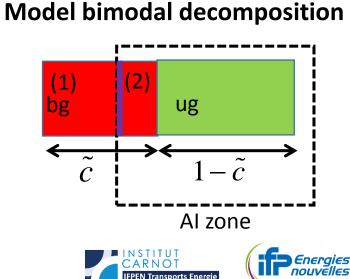
$$\Phi\Big|^{ai} = (1 - \tilde{c}_{ai}) \Phi\Big|^u + \tilde{c}_{ai} \Phi\Big|^b$$

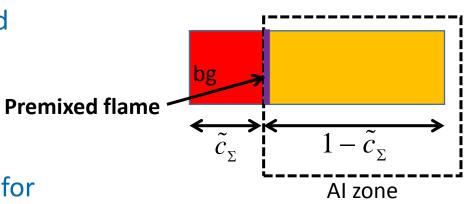
• Total burned gases fraction  $\tilde{c}$  is then given by:



#### Real bimodal decomposition

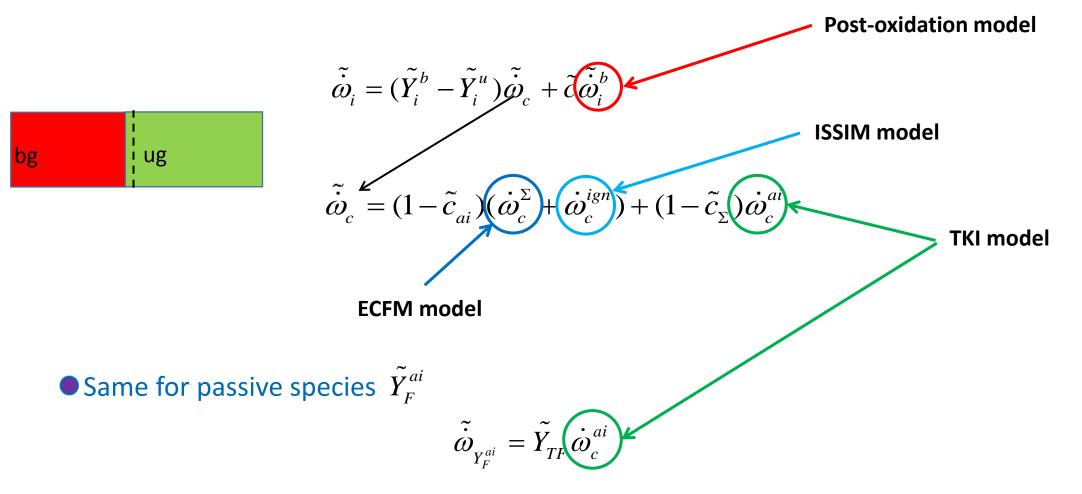
SUSTAINABLE MOBILITY





# SPECIES SOURCE TERMS







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# TKI TABLE GENERATION WITH KICGEN AND USAGE

#### Choice of a mechanism

- Single component (ex: n-heptane)
- multi-component with fixed composition (ex: 70% n-heptane + 30% iso-octane)

#### • Exemples:

	Number of species	Number of reactions
Anderlohr et al. [4]	536	3000
<u>Chalmers</u> [17,18]	42	168
Zeuch et al. [11]	121	593

#### Choice of the parameter range

Exemple:	min	max	total number
FAER	0.1	3	9
Pressure (bar)	1	200	12
Temperature	500	1500	56
EGR(%)	0	80	4
Progress variable c	0	1	99

#### 24192 kinetic calculations

#### **KicGen**

- Kinetic mechanism
- Range of parameters
- Generate input files for SAGE

#### SAGE

• Full parallel 0-dimensional SAGE homogeneous calculations

#### KicGen

- Check calculations
- Progress variable postprocessing
- Write TKI hdf5 table

#### **TKI table ready**

#### CONVERGE

- Reads TKI table at run start
- ECFM3Z interpolates in TKI table in each cell at each time-step

# $\dot{\omega}_{c}^{ai}(x,t) = \dot{\omega}_{c}^{TKI}(P,\tilde{T}_{u},\bar{\Phi},X_{dil},c_{ai})(x,t)$





#### TKI REACTION RATE CALCULATION [1,2]

Algorithm for one thermodynamic condition

- Calculation of a constant pressure homogeneous reactor using any complex mechanism with a kinetic solver (Sage, etc...)
- Progress variable defined as the normalized reactor temperature

 $T_{\cdot} - T_{\circ}$ 

$$c_i = \frac{r_0}{T_N - T_0}$$

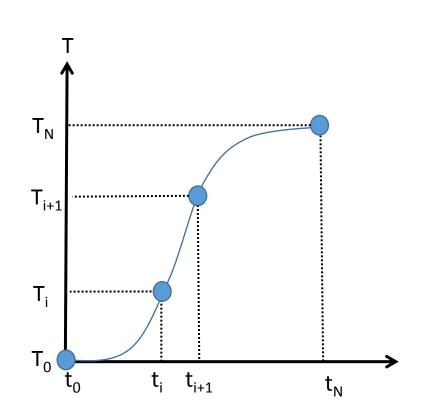
• TKI reaction rate defined as the progress variable derivative

$$\dot{\omega}_{c}^{TKI}(c_{i}) = \frac{c_{i+1} - c_{i}}{t_{i+1} - t_{i}}$$

Repeat for all thermodynamic conditions

$$\dot{\omega}_{c}^{ai} = \dot{\omega}_{c}^{TKI}(P, \tilde{T}_{u}, \bar{\Phi}, X_{dil}, c_{ai})$$



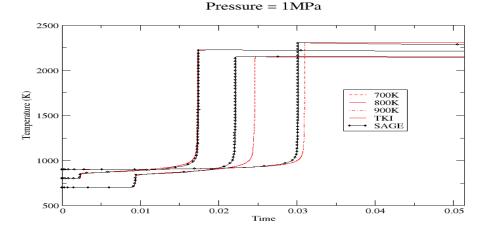


[1] Colin et al., PCI, 2004

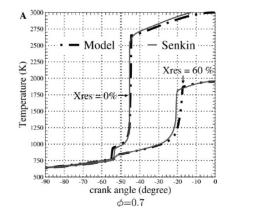
[2] Robert et al., PCI, 2015

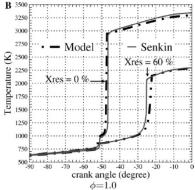


Constant pressure homogeneous reactor case Comparison with kinetic solver simulations



### Variable volume homogeneous reactor case Comparison with kinetic solver simulation [1]







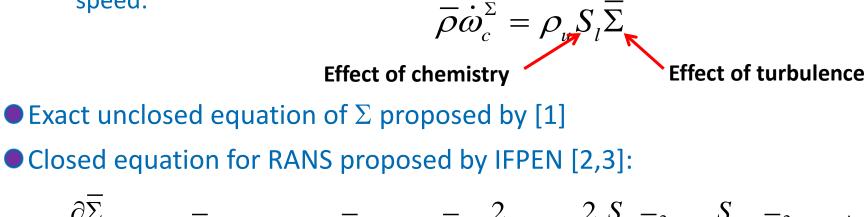


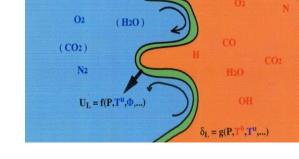
#### **ECFM MODEL**

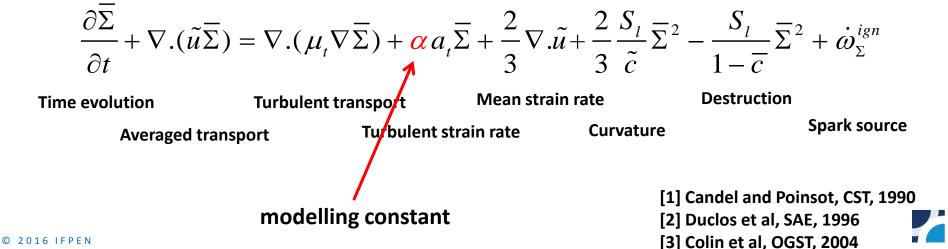
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- Based on the flamelet assumption
  - flame thickness smaller than all turbulent scales
  - Iccally, the flame is identical to a laminar flame propagating at the laminar flame speed S<sub>I</sub>

• Reaction rate is thus the product of the flame surface density  $\Sigma$  (=S/V) by the laminar flame speed:







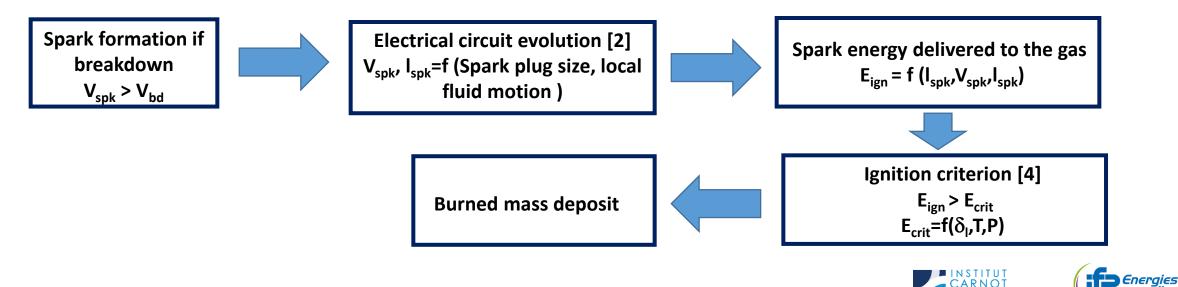
## **ISSIM MODEL[1]**

[1] Colin and Truffin, PCI, 2011[2] Duclos and Colin, Comodia, 2000[3] Adelman, PCI, 1981

SUSTAINABLE MOBILITY

Transports Energ

- Provides spark plug ignition source terms in  $\Sigma$  and species equations
- It accounts for various phenomena :
  - Electrical circuit model
  - Local mixture properties (fuel/air ratio, temperature etc...) at the spark plug
  - Effect of convection on the initial kernel
  - Effect of turbulence of kernel wrinkling
- Electrical circuit description[2]

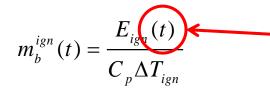


## **ISSIM MODEL SOURCE TERMS[1]**

[1] Colin and Truffin, PCI, 2011
[2] Duclos and Colin, Comodia, 2000
[3] Erweg and Maly, SAE, 1992
[4] Mulla et al, CF, 2016

#### SUSTAINABLE MOBILITY

#### Initial burned gases mass deposition proportional to electrical energy in gas



Eign increases with time as long as arc exists =>mbign also increases (flame holder effect[3])



Distribution of the initial burned gases mass on a Gaussian profile centered on eletrodes gap

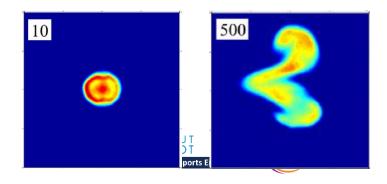
$$\overline{c}_{ign}(x,t) = \frac{m_b^{ign}(t)\exp(-r^2/\delta_{spk}^2)}{\int \exp(-r^2/\delta_{spk}^2)dV}$$

• Species and  $\Sigma$  source terms

$$\dot{\omega}_{c}^{ign} = \max(\overline{c}_{ign} - \overline{c}, 0) / dt$$
$$\dot{\omega}_{\Sigma}^{ign} = \max(\Xi_{ign} \frac{3}{r_{ign}} \overline{c}_{ign} - \overline{\Sigma}, 0) / dt$$

modelling constant= initial flame wrinkling Sources of initial wrinkling:

- Toroidal shape of the kernel due to chock wave [4]
- Flow around spark plug
- Plasma dynamics



### **BURNED GASES REACTIONS**

• Major species reaction rate (Fuel, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, H, O, OH)

Given by simplified two-step reaction mechanism + radicals equilibrium computation

$$C_x H_y + (\frac{x}{2} + \frac{y}{4})O_2 \rightarrow xCO + \frac{y}{2}H_2O$$

• Allows:

• Generic fuel oxidation for non-premixed combustion (Diesel or very rich zones in SI engines)

Correct estimation of burned gases composition => correct Tb and CO/CO2 ratio

 $CO + \frac{1}{2}O2 \longrightarrow CO2$ 

Does not allow:

• Fuel formulation impact on reaction rate

Minor species prediction (HC)

Pollutants reaction rate (passive species formulation)

- Zel'Dovitch NO mechanism [1] (thermal NO model)
- Hiroyasu soot model from Converge [1] (semi-empirical soot model)



### ECFM3Z CALCULATION PROCEDURE

- fuel surrogate definition
  - Mean fuel formulation: CxHyOz
  - Thermodynamic data (liquid and gas)
- TKI table
  - Use existing table (available from CSI)
  - Or generate table with KicGen (need mechanism)
- Laminar flame speed
  - Set SI correlation parameters in combust.in
  - Or use UDF table
- Set ISSIM parameters in issim.in (spark timing, ignition energy etc...)
- Set ECFM3Z parameters in combust.in (factor  $\alpha$  etc...)
- Set correct species and passives for ECFM3Z
- Run Converge
- Specific ECFM3Z outputs in passive.out, ecfm3z.out and issim\_ignition\_0.out



# OUTLOOK OF THE PRESENTATION

The ECFM3Z combustion model

Diesel application

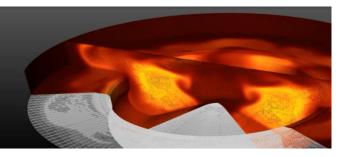
• SI application

• Future developments in Converge





#### PASSENGER CAR DIESEL ENGINE DATABASE



#### Experimental database (provided by Renault SA) :

- •40 operating points, 10 calculated
- Load and high load
- Engine speed (rpm) variation (1500rpm, 4000rpm)
- EGR rate variation at low load (0%,15%,30%)
- Start of Injection (SOI) variation (full and partial load)

#### Renault Diesel Engine

Number of cylinder	1
Compression ratio	14.8:1
Engine bore	0.084m
stroke	0.09m
Connective rod length	0.1435m
Number of holes	6
Nozzle diameter	155µm



# MESH RESOLUTION STUDY

- Aim: find the correct settings of AMR, embedding and dx\_base to ensure mesh convergence
  - Wedge mesh (1/6th)
  - Compression and expansion only

	Α	В	С	D	E		Cells min	5k	7k	38k	18k	34k
							Cells max	46k	180k	420k	960k	3600k
Dx base	2.8	1.4	0.7	1.4	1.4							
							Number of	70k	100k	500k	500k	800k
Embed scale	2	2	2	3	4		Parcels					
Dx min	0.7	0.35	0.175	0.175	0.0875		Simulation	1.000		52.452	20500	0.001.00
							return time (16 cores)	1680	6600	52452	38598	260140
		A - B C - D E			300 - 250 - (300 - 250 - 150 - 50 - 0 - 0 - 0 -	5 Crank a		ise A lise B lise C lise D lise E		B is a go	neshes a bod comj n CPU ar	re converged



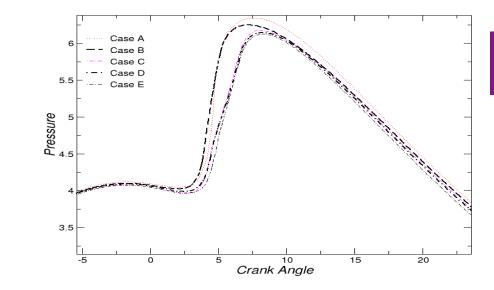
Energies nouvelles

# MESH RESOLUTION STUDY

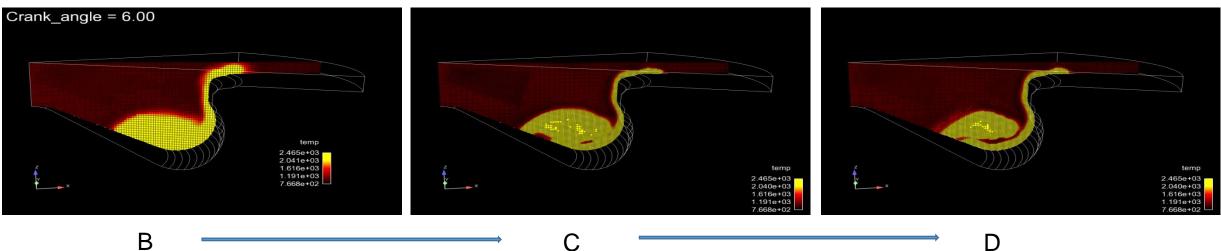
#### • Comparison of temperature and pressure for different meshes

	Α	В	С	D	Е
Dx base	2.8	1.4	0.7	1.4	1.4
Embed scale	2	2	2	3	4
Dx min	0.7	0.35	0.175	0.175	0.0875

#### Temperature in cut plane



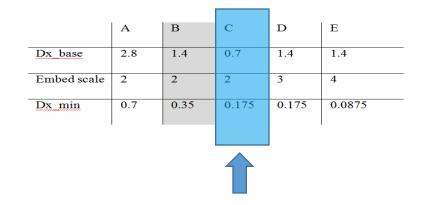
Cylinder pressure



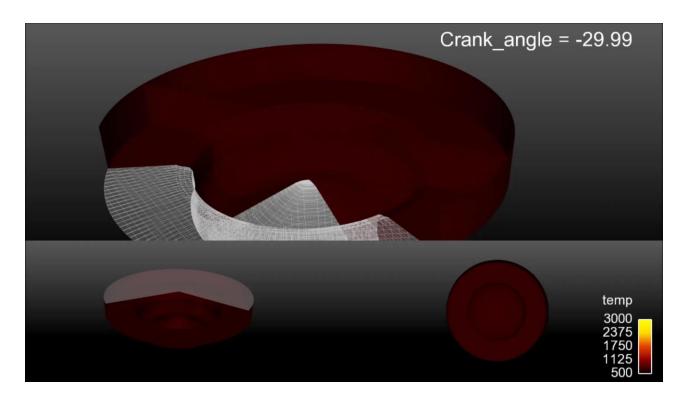


# MESH RESOLUTION STUDY

#### SUSTAINABLE MOBILITY



- Embedded zone around the spray
- AMR on temperature / velocity
- Set AMR to C case
- ECFM3Z with the Anderlhor kinetic mechanism



Temperature field

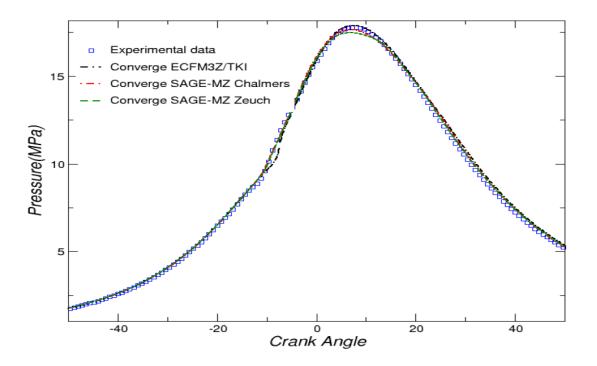


# CPU TIME OF ECFM3Z COMPARED TO SAGE

#### SUSTAINABLE MOBILITY

#### • Mesh B is used

- Very similar results between ECFM3Z and Sage
- CPU cost reduction by 3.5 to 11 with ECFM3Z compared to Sage with multi-zone enabled



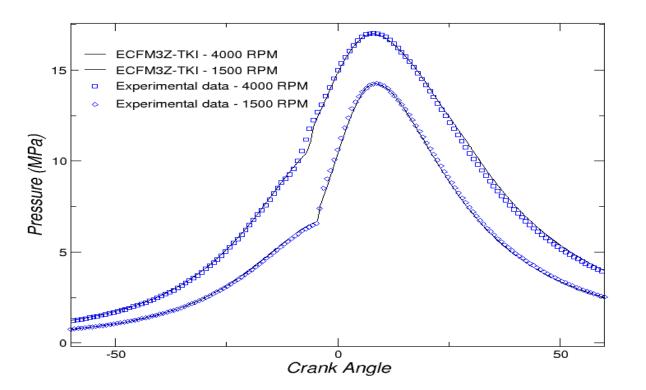
	А	В	С	D	Е
Dx base	2.8	1.4	0.7	1.4	1.4
Embed scale	2	2	2	3	4
Dx min	0.7	0.35	0.175	0.175	0.0875

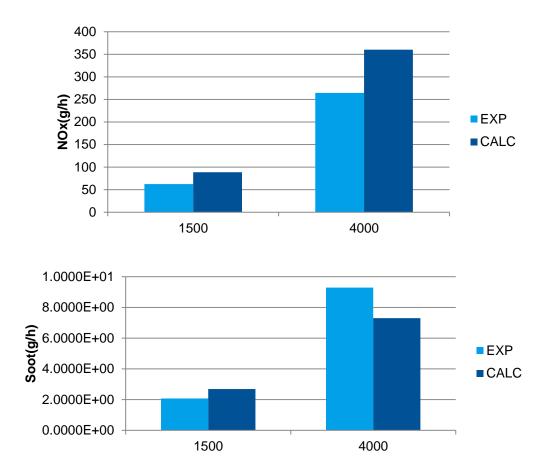
		Number of species	Number of reactions		
	Anderlohr et al. [4]	536	3000		
	Chalmers [17,18]	42	168		
	Zeuch et al. [11]	121	593		
		Normalized Simulation time			
ECFM.	3Z/TKI Anderlohr	1			
SAGE	MZ Chalmers	3.43	3		
SAGE	MZ Zeuch	10.8	10.84		



#### 1500 and 4000 rpm at full load

Good prediction of pressureGood NOx and soot prediction



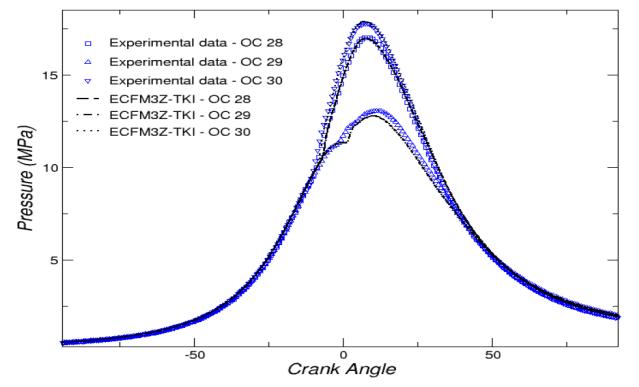


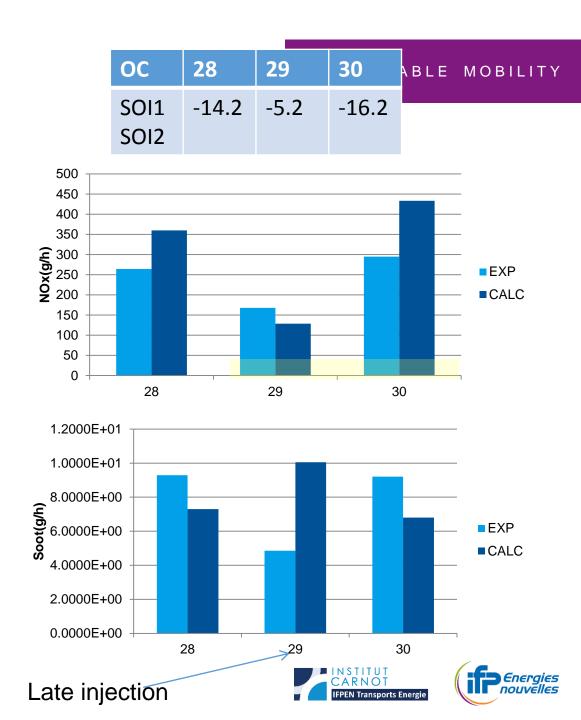
IN STITUT CARNOT IFPEN Transports Energie

#### SUSTAINABLE MOBILITY

### 4000 rpm at full load – SOI variation

- Good pressure prediction
- Reasonable NOx and soot prediction
- Difficulty for late injection case

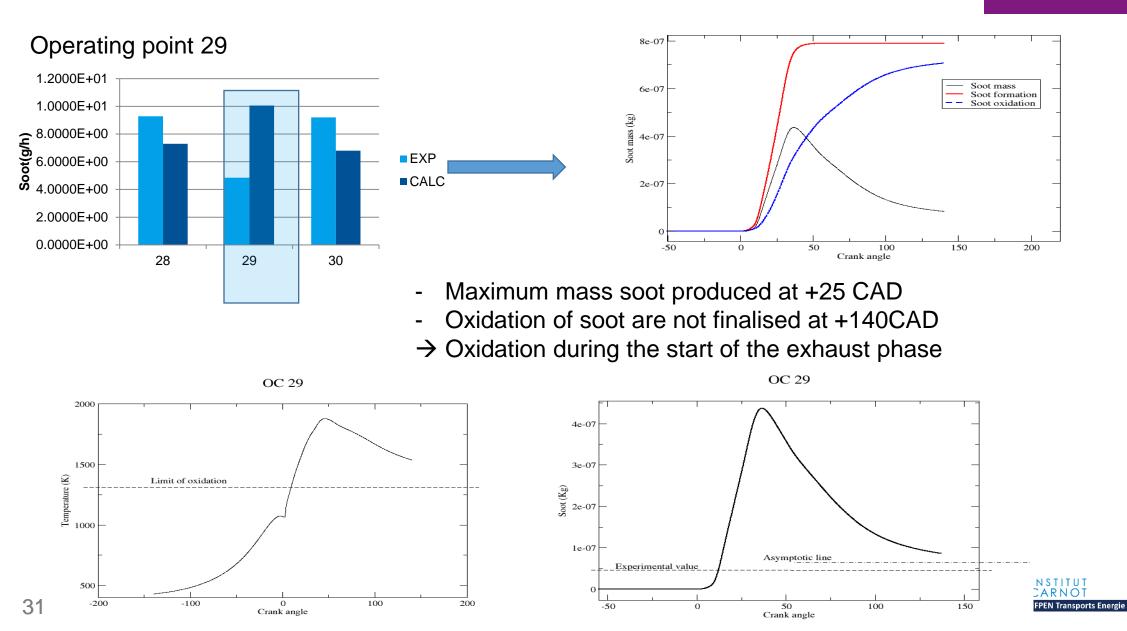




#### SUSTAINABLE MOBILITY

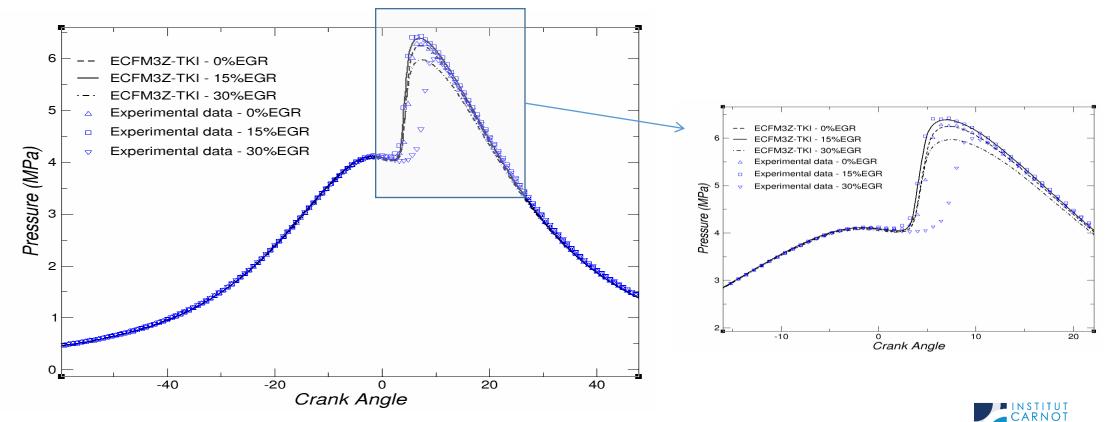
Energies

nouvelles



#### 1500 partial load – EGR variation

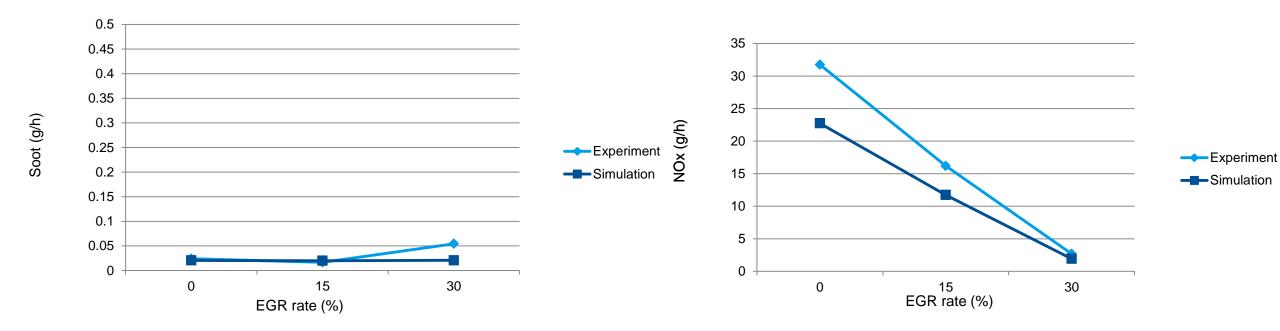
- Good prediction of pressure for 0 and 15% cases
- Under-prediction of auto-ignition delay for 30% case (possible causes: mechanism, strain effect)



Transports Energy

#### **1500 partial load – EGR variation**

- Good prediction for NOx
- Soot increase at 30% not reproduced





# OUTLOOK OF THE PRESENTATION

The ECFM3Z combustion model

Diesel application

• SI application

• Future developments in Converge





### EXPERIMENTAL SET UP AND METHODOLOGY

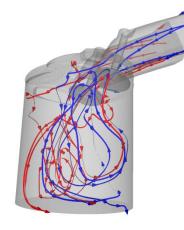
#### ICAMDAC single cylinder engine

- Description
  - Experimental set up dedicated to abnormal combustion study
  - Representative of an up to date SI engine (turbocharged, direct injection)
  - Two experimental devices : optical engine and full metal engine

#### • Optical engine



- High frequency sensors
- PIV visualization



#### • Full metal engine

- High frequency sensors
- Combustion analysis

SUSTAINABLE MOBILITY

- Numerical set-up definition
- Fluid motion comparisons

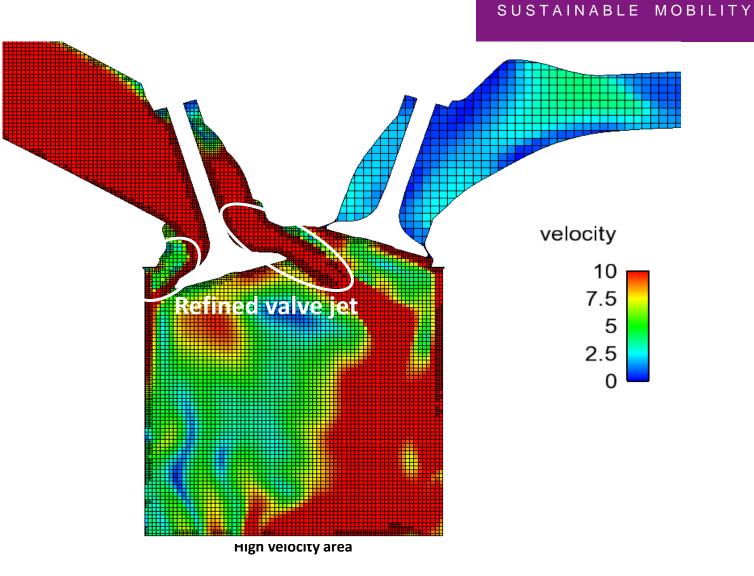
→One operating point :

- engine speed 1800rpm IMEP 19 bar
- Model calibration
- Combustion comparisons
   Five operating points :
  - engine speed 1800rpm IMEP 19 bar
  - engine speed 1200rpm IMEP 20 bar
  - engine speed 4000rpm IMEP 19 bar
  - engine speed 1200rpm IMEP 6 bar
  - engine speed 3000rpm IMEP 6 bar

## **OPTICAL ENGINE**

#### • Numerical setup validation

- Embedding area
- AMR levels
- Turbulent model



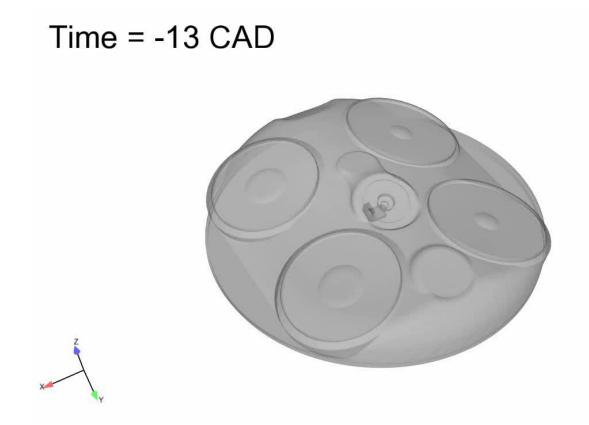


# FULL METAL ENGINE

SUSTAINABLE MOBILITY

# ECFM3Z simulation

• 1800rpm 19 bar operating point with spark timing set at the knock limit

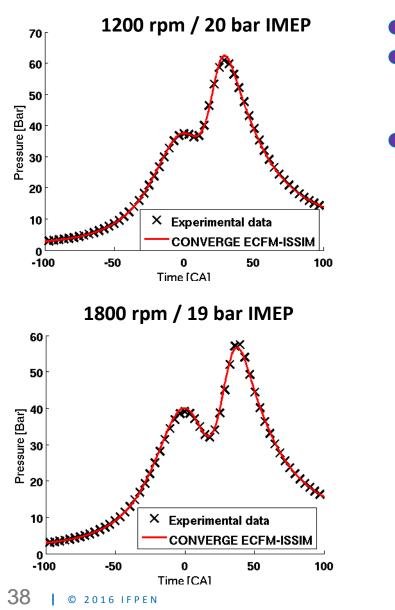


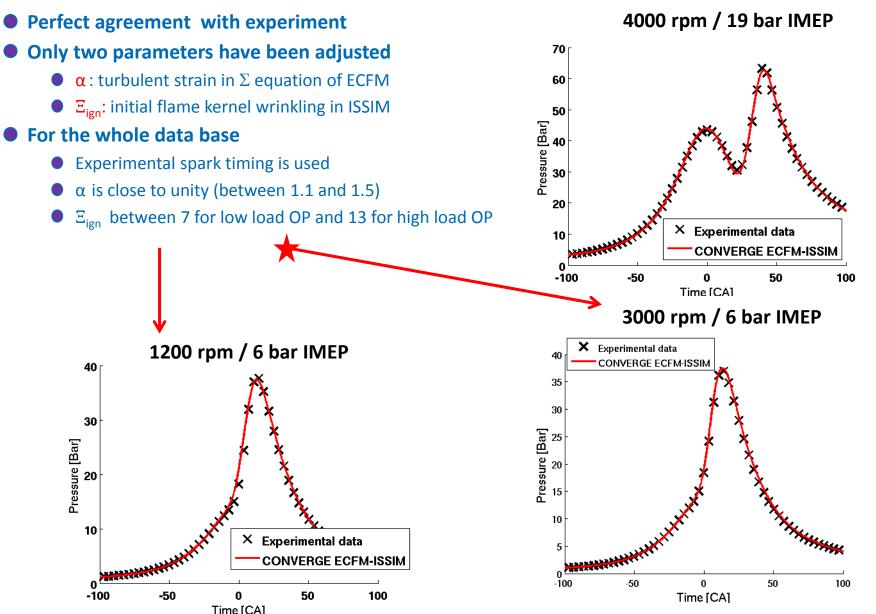
• ECFM approach allows to record the flame front displacement



# **ECFM VALIDATION**

#### SUSTAINABLE MOBILITY

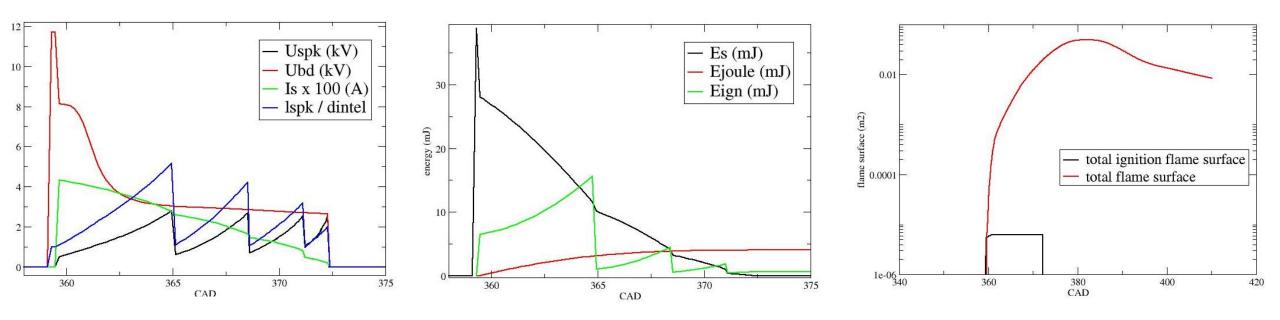




#### Current and voltage

#### Electrical energy

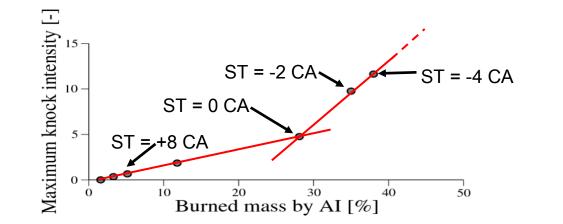
#### • Flame surface





# KNOCK VALIDATION METHODOLOGY

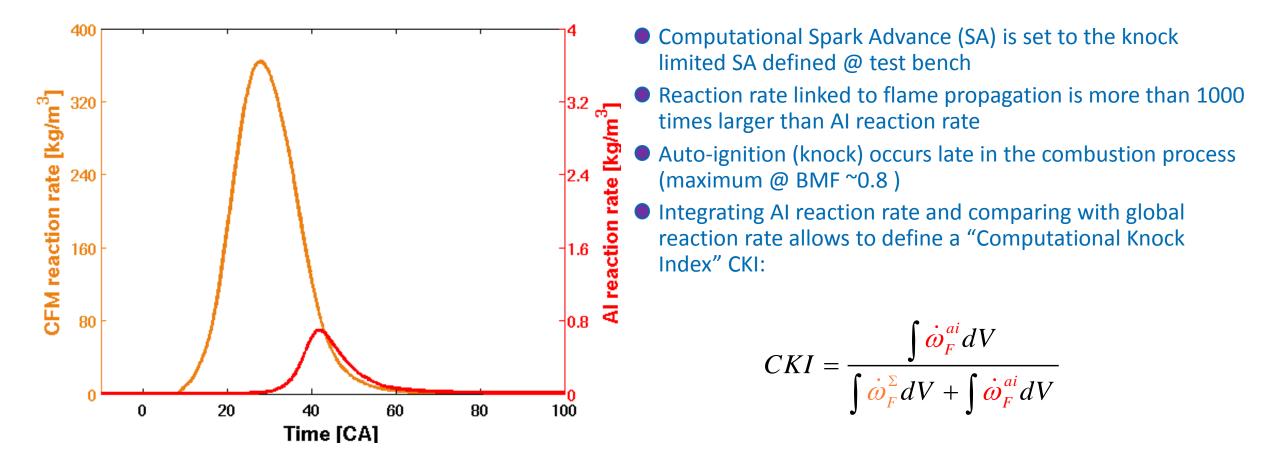
- Direct comparison of pressure with experiments is difficult
  - At test bench knock detection is performed recording pressure and applying high pass filter to get pressure fluctuations
  - In LES, these pressure fluctuations could be reproduced [1]
  - In RANS, pressure fluctuations are damped because:
    - the mean fresh gases mass given by RANS is much smaller than the instantaneous fresh gases mass of a knocking cycle=> the pressure fluctuation will be under-predicted
    - Iarge time-step (to save CPU time) tend to damp pressure fluctuations
- It was shown in LES that the fresh gases mass burned by auto-ignition is proportional to the experimental knock index [1]
  - This fact is used here to define a Computational Knock Index that can help determining the knock limit



[1] Robert et al. , PCI, 2015



# • Premixed and AI HRR for the 1800rpm/19bar OP



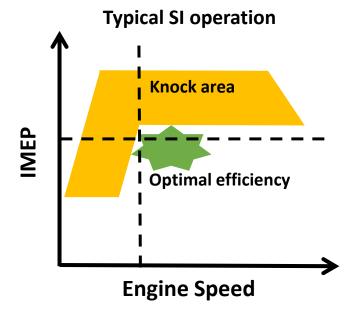


# The goal is to check if ECFM and TKI models are able to reproduce main trends concerning knock with the CKI

@ iso –Engine speed :

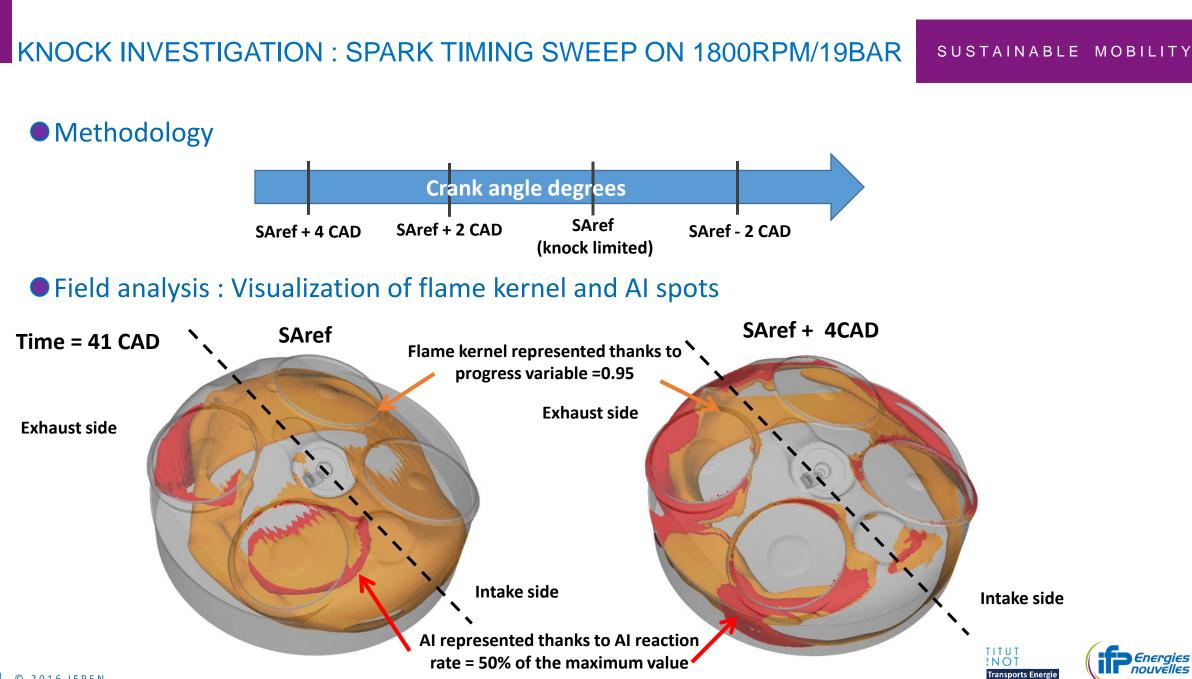
- Knock intensity increases with the load

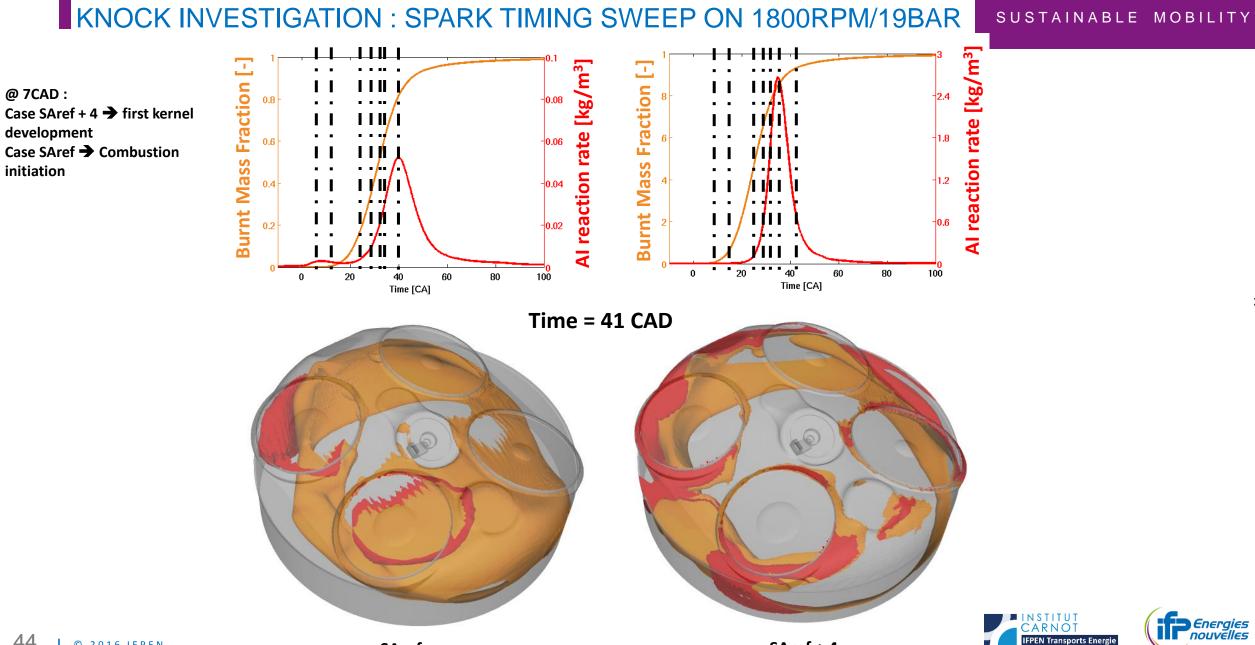
- Higher loads lead to tougher thermodynamic conditions which reduces AI delays



- @ iso -IMEP :
- Knock intensity decreases with engine speed
- Larger engine speed leads to lower residence time and therefore lower AI



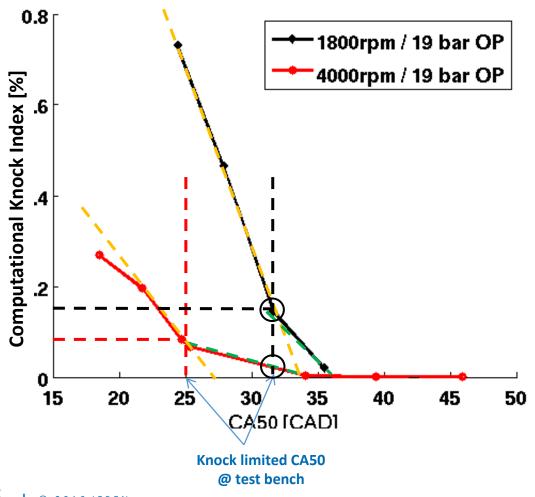




:

# ANALYSIS OF CKI : DEPENDENCY TO ENGINE SPEED

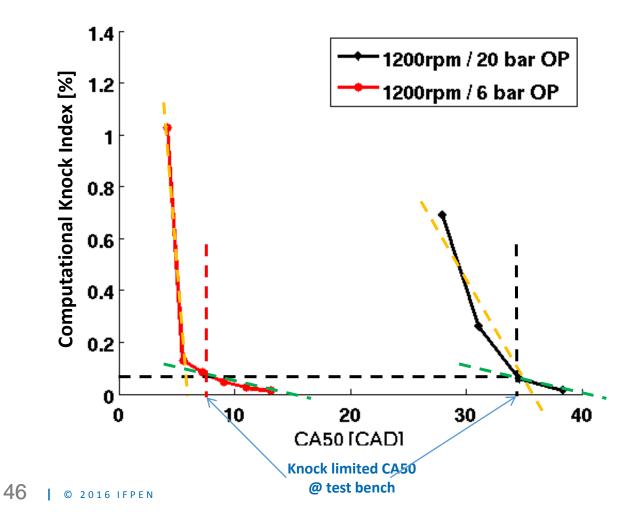
### Comparison between 1800rpm/19bar OP and 4000rpm/19bar OP



- Low increase of CKI at large CA50 like in experiment
- Steep increase of CKI close to experimental knock limited CA50
  - CKI recovers qualitatively the knock limit
- Larger value of CKI at knock limit for low engine speed
  - Expected result: longer residence time at low engine speed
     =>more time to auto-ignite
  - A single value of CKI cannot be defined for the whole map
  - A more complex index needs to be defined in the future
- Sensitivity of knock to SA is larger at low engine speed (i.e. slope is steeper for 1800rpm OP)
- Results fully coherent with experimental observations



# **Comparison between 1200rpm/6bar and 1200/20bar operating points**



- High load OP
  - Low increase of CKI at large CA50 like in experiment
  - steep increase of CKI close to experimental knock limited CA50
  - CKI recovers again the knock limit qualitatively
  - Value of CKI again different from other high load operating points
- Low load OP
  - slope of CKI remains low at experimental optimal CA50
  - means that CKI recovers that this OP is not limited by knock
  - strong knock (i.e. slope steepening) is observed after the optimal CA50



# ANALYSIS OF CKI: HIGH LOAD LIMIT

#### • CKI varies with engine speed at high load

	1200rpm/20bar	1800rpm/19bar	4000rpm/19bar
Optimal exp. CA50	32	32	25
CKI at opt.exp. CA50	0.26	0.15	0.08

#### • CKI x rpm is nearly constant for three high load points

 Indicates a new definition of a computational knock index based on HRR by auto-ignition could work better



# CPU TIME FOR SI ENGINE

# • Low CPU time for a complete cycle

case	1200rpm/20bar	4000rpm/19bar
Elapsed CPU time (on 32 procs)	31h	22h

#### • Low mesh resolution requirement

- Base grid in the cylinder: dx = 0.5mm
- Refinement at spark plug and walls: dx=0.25mm



# OUTLOOK OF THE PRESENTATION

The ECFM3Z combustion model

Diesel application

• SI application

• Future developments in Converge





# • Available in V2.3.16

- ECFM3Z as described in this presentation
- ISSIM
- TKI and KicGen generator (contact CSI for table generation)
- Simple NOx and soot models

# Short term developments

- Multi-fuel description in ECFM3Z and TKI
  - Allows better fuel evaporation and auto-ignition description (multi-component)
- Simple dual-fuel flame surface density source term
  - Allows dual fuel calculation (e.g. Diesel fuel + natural gas)



#### • Longer term developments

- ADF-TKI for Diesel: improved TKI model accounting for effect of strain on auto-ignition [1]
  - Improved lift-off length
  - Improved auto-ignition delays at low loads (cases with long ignition delays)
- Kinetic solver in burned gases (Sage)
  - Effect of fuel formulation on HRR
  - Minor species prediction enabled (HC)
  - PAH description (for soot)
- Sectional soot model coupled to ECFM3Z
  - Better prediction of soot mass and number (Diesel and gasoline)
  - Access to soot size distribution
- High Karlovitz ECFM model
  - Better prediction of premixed flame HRR at high turbulence and EGR rates



# CONCLUSIONS

• ECFM3Z fully revised by IFPEN now available in Converge

#### Diesel engine simulations

- Good prediction of pressure and pollutants
- Low CPU times compared to Sage

# Gasoline engine simulations

- Very good prediction of pressure with minor parameters adjustment
- Good ability to predict knock occurrence with proposed computational knock index
- Low CPU times compared to other models

• Further model improvements to come in a long term collaboration with CSI





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