

# Simulation of accelerated deflagrations with the CALIF<sup>3</sup>S-P<sup>2</sup>REMICS software using RANS and LES approaches

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## Background & Motivations

### □ Safety issues related to explosion hazards

- ⇒ in case of severe accident in the reactor building,
- ⇒ inside or outside the reactor building in case of loss of sealing of pipes containing hydrogen.



Explosion at Fukushima reactor 3



Hydrogen jet deflagration

→ The IRSN develops an in-house software for the simulation of explosions: CALIF<sup>3</sup>S-P<sup>2</sup>REMICS.

## Background & Motivations

- ❑ Models currently used in CALIF<sup>3</sup>S-P<sup>2</sup>REMICS for deflagrations:
  - ➔ Turbulence: RANS approach,
  - ➔ Combustion: turbulent flame-speed closure combustion model.
- ❑ Drawbacks of this approach:
  - ➔ Rough description of the turbulence,
  - ➔ Results strongly dependent on the turbulent flame speed correlation.
- ❑ Difficulties:
  - ➔ Lack of experimental data for the validation of turbulence models,
  - ➔ Cost of the experiments, variability of the configurations encountered, need for change of scale...

### → Development of a LES approach for deflagration

- ❑ Objective: use LES approach in order to
  - ➔ Obtain predictive and detailed data on turbulence,
  - ➔ Improve the RANS approach.

[Bray, 1990] correlation



[Peters, 2000] correlation



[Zimont, 2000] correlation



Volvo test rig: fuel mass fraction

## Outline

### **Combustion models**

LES approach

RANS approach

### **An accelerated deflagration**

Experimental setup

### **LES numerical results**

Influence of obstacles location

Constant vs dynamic wrinkling factor exponent

### **RANS numerical results**

### **Summary & Perspectives**

## LES approach

- A virtually thickened flame formalism (TFLES) is used [Butler & O'Rourke, 1977]
  - ⇒ The flame thickness is increased by a factor  $\mathcal{F}$  while keeping the laminar flame speed  $s_l$  constant.
- Increasing the flame thickness induces a reduced sensitivity of the flame to turbulent motions:
  - ⇒ Eddies of size smaller than  $\mathcal{F} \delta_l^0$  cannot wrinkle the thickened flame front, with  $\delta_l^0$  the laminar flame thickness,
  - ⇒ A wrinkling factor  $\Xi_\Delta$  for the sub grid scales is introduced.

Chemical species balances:

$$\partial_t \overline{\rho y_k} + \text{div}(\overline{\rho y_k \tilde{u}}) + \text{div}(\mathcal{F} \overline{j_k}) = \frac{\overline{\dot{\omega}_k}}{\mathcal{F}}$$

Sensible energy balance:

$$\partial_t(\overline{\rho \tilde{e}}) + \text{div}(\overline{\rho \tilde{u} \tilde{e}}) + \overline{p} \text{div}(\tilde{u}) + \text{div}(\mathcal{F} \overline{q}) = \frac{\overline{\dot{\omega}_T}}{\mathcal{F}} + \overline{\tau}(\tilde{u}) : \nabla \tilde{u} + \epsilon_v$$

1/2



DNS of flame turbulence interactions



Flame artificially thickened by a factor  $\mathcal{F}$

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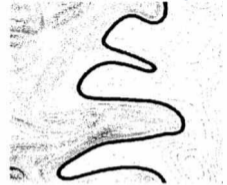
Chemical species balances:

$$\partial_t \overline{\rho y_k} + \text{div}(\overline{\rho y_k \tilde{\mathbf{u}}}) + \text{div}(\Xi_\Delta \mathcal{F} \overline{\mathbf{j}_k}) = \Xi_\Delta \frac{\overline{\dot{\omega}_k}}{\mathcal{F}}$$

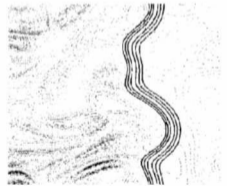
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## LES approach

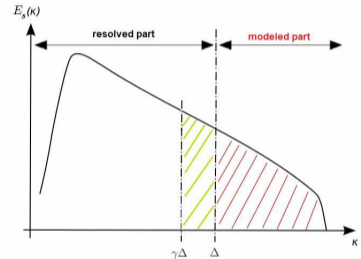
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- The [Veynante & Moureau 2015] formulation is used for the subgrid scale wrinkling factor  $\Xi_{\Delta}$ :

$$\Xi_{\Delta} = \left( \frac{\Delta}{\delta_c} \right)^{\beta}$$

$\Delta$  being the combustion filter size,  $\delta_c$  the inner cutoff scale (*i.e.* the lowest wrinkling scale).

- The model parameter  $\beta$  can be:
  - fixed,
  - dynamically determined equating flame surfaces computed at filtered and test-filtered scales (Germano-like identity),
  - corrected in order to take into account flame front interactions and flame/wall interactions [Mouriaux, 2011]
    - avoid unphysical values of the subgrid scale wrinkling factor.



Germano-like procedure: resolved scales are used to model subgrid scales

## LES approach

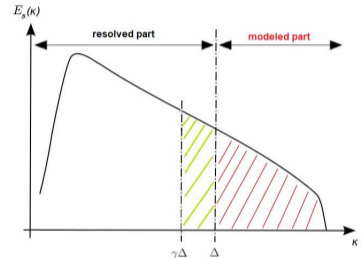
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Germano-like procedure: resolved scales are used to model subgrid scales



## RANS approach

- Geometrical description of the flame front (G-equation, [Peters, 2000]):

$$\partial_t(\bar{\rho} \tilde{G}) + \text{div}(\bar{\rho} \tilde{G} \tilde{\mathbf{u}}) + \rho_u u_f |\nabla \tilde{G}| = 0$$

- but, for partially premixed flow,  $G$  cannot be identified to a progress variable...  
↪ keep the usual mass balance equations for the chemical species, and compute the reaction rate as a function of  $G$ :

$$\bar{\omega} \sim \rho_u \frac{u_f}{\delta_F} \max\{0.5 - \tilde{G}, 0\} \eta(\tilde{y}_F, \tilde{y}_O).$$

homogeneous to a length  $\downarrow$  guarantees that  $y_F, y_O \geq 0$   
 $\downarrow$   
 $\dot{\omega} = 0$  in fresh gases,  $\dot{\omega} \gg 1$  in burnt gases

- The turbulent flame speed  $u_f$  is given by correlations (Zimont, Peters,...):

$$u_f = f(s_l, u', l_t, \dots),$$

and the laminar flame speed is defined from unburnt mixture local conditions:

$$s_l(\phi, p, \theta) = s_l^{\text{ref}}(\phi) \left( \frac{T}{T_{\text{ref}}} \right)^\alpha \left( \frac{p}{p_{\text{ref}}} \right)^\beta.$$

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## An accelerated deflagration - Experimental setup

### □ Context:

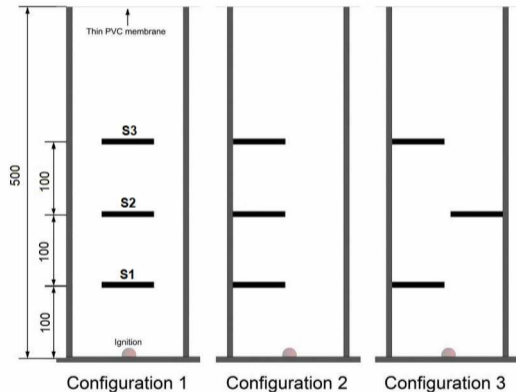
- ➡ Accelerating flame in an obstructed square channel.

### □ Geometry [Wen *et al.*, 2013]:

- ➡ Obstructed semi-confined chamber (150 mm × 150 mm × 500 mm),
- ➡ Top of the chamber sealed with a thin polyvinyl chloride membrane,
- ➡ Three configurations of obstacles (75 mm × 150 mm × 10 mm).

### □ Configuration:

- ➡ Stoichiometric methane-air mixture,
- ➡ Ignition at the bottom of the chamber.



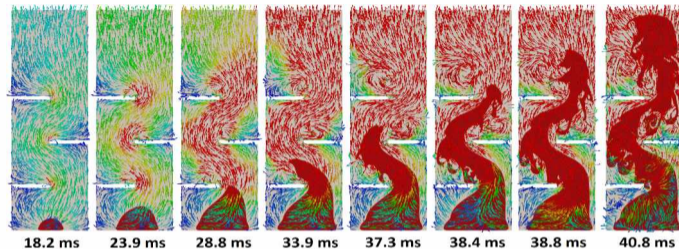
## LES numerical results

- ❑ 2D numerical results are performed in order to setup 3D simulations.
- ❑ 3D simulations have been performed on the supercomputer Topaze at the Research and Technology Computing Center (CCRT).
- ❑ 3D numerical results confirm the results obtained in 2D.
- ❑ Only 2D numerical results are presented here.

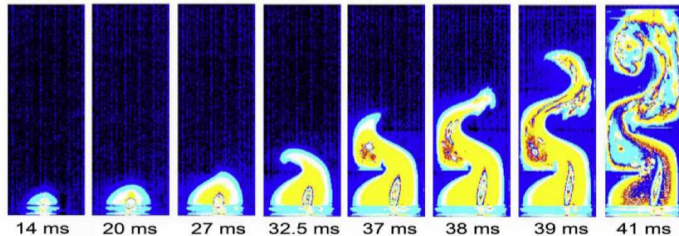


Image of the flame front  
(3D simulations)

### Configuration 3: flame front structure

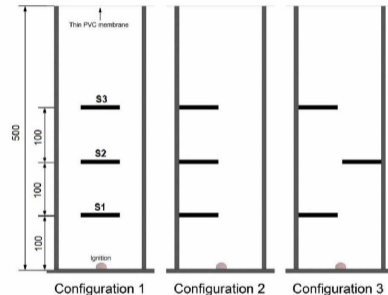
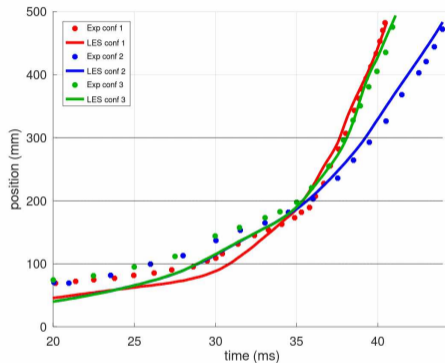


Snapshots of the temperature field and velocity vectors



Experimental images

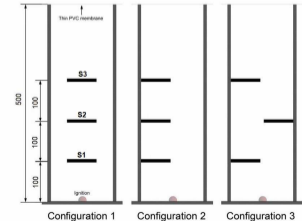
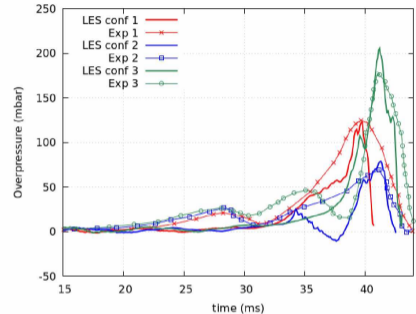
## Influence of obstacles location - Flame front position



- The transition from laminar to turbulent well recovered (before the first obstacle)
- Good reproduction of the flame acceleration, but flame faster than experiments between the first and the second obstacles
- Staggered obstacles configuration: faster flame.

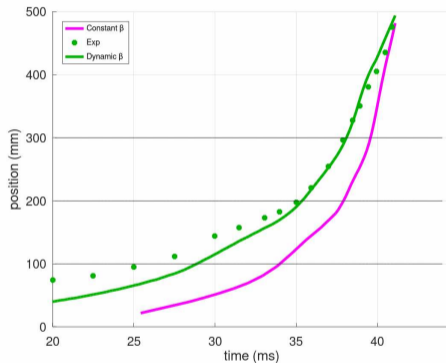
## Influence of obstacles location - Overpressure evolution

- ❑ First experimental peak due to sealing film disintegration: not simulated, thus not recovered.
- ❑ Configurations 1 and 2:
  - ➡ Overpressure peaks reached when the flame front is located between the third obstacle and the exit,
  - ➡ Overpressure peaks well recovered.
- ❑ Configuration 3:
  - ➡ Overpressure peak reached when the flame front is located outside the chamber,
  - ➡ Overpressure peaks overestimated.
- ❑ Staggered obstacles configuration: most penalizing.

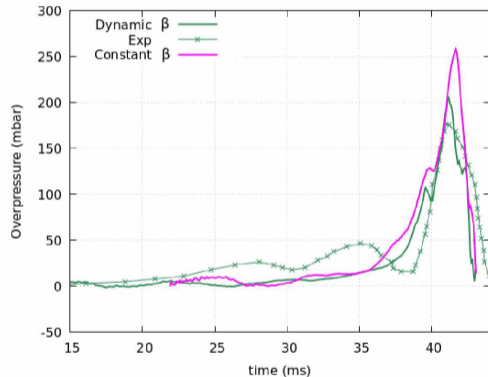


## Configuration 3 - Constant vs dynamic wrinkling factor exponent

Flame front position



Overpressure evolution



- ❑ Numerical results obtained with a fixed or dynamically computed wrinkling factor are compared.
- ❑ The dynamical formulation of the wrinkling factor is essential to catch the transition from laminar to turbulent regimes and recover the good flame behaviour.



## RANS numerical results - Modelling

□ Turbulence:  $k$ - $\omega$  SST model,

□ Combustion: turbulent flame-speed closure combustion model

- [Bray, 1990] correlation:  $u_f = 0.875 \text{Ka}^{-0.392} u'$ , with  $\text{Ka} = 0.157 \left(\frac{u'}{s_l}\right)^2 \text{Re}_T^{-0.5}$ ,

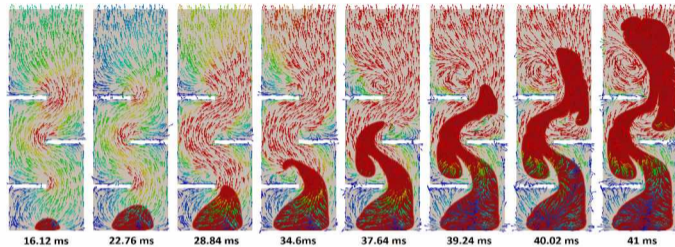
- [Zimont, 2000] correlation:  $u_f = A u' \text{Da}^{1/4}$ ,

- [Goulier, 2015] correlation:  $u_f = s_l 1.613 \left(\frac{r}{l_t}\right)^{0.333} \left(\frac{u'}{s_l}\right)^{0.526} \text{Le}^{-0.14}$ .

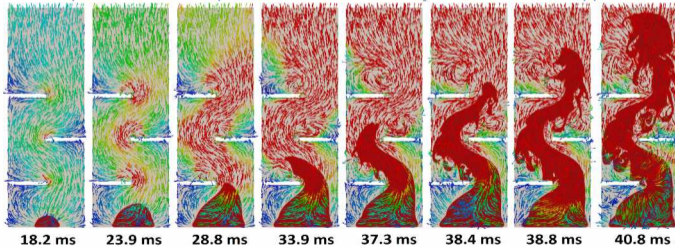
→ Numerical simulations are performed on a 2D computational domain with the three turbulent flame speed correlations.

→ Only configuration 3 (staggered obstacles) is simulated.

## Flame front structure (RANS vs LES) - Goulier correlation

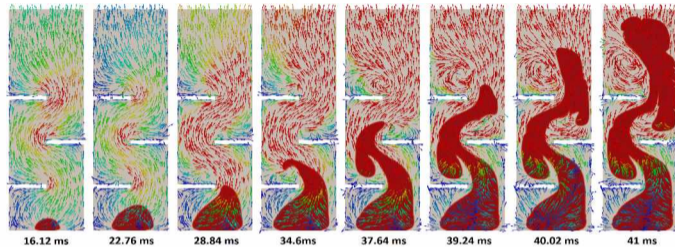


Snapshots of the temperature field and velocity vectors - RANS approach

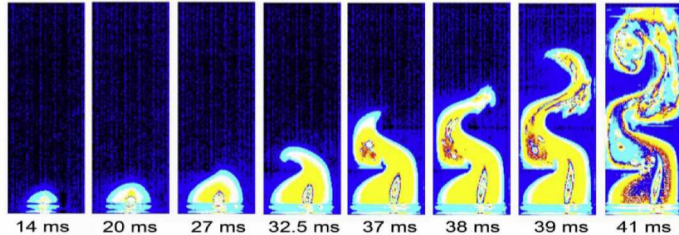


Snapshots of the temperature field and velocity vectors - LES approach

## Flame front structure (RANS vs Experiment) - Goulier correlation



Snapshots of the temperature field and velocity vectors



Experimental images

# Turbulent flame speed correlation impact

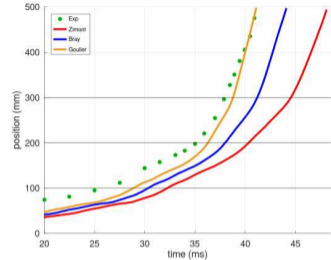
## Flame front position:

- ➡ Goulier correlation: good approximation of the flame front position,  
→ the transition from laminar to turbulent flame is well reproduce probably due to the term  $(r/l_t)^{0.333}$  [Gostintsev *et al.*, 1988].
- ➡ Zimont and Bray correlations: underestimation of the flame speed  
→ these correlations are designed for situations where the turbulence is fully developed.

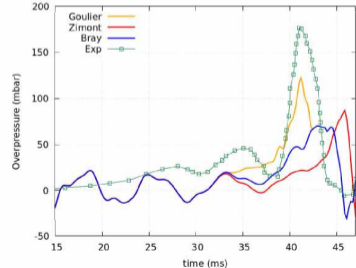
## Overpressure evolution:

- ➡ Underestimation of the pressure peak with the three correlations,
- ➡ Pressure fluctuations due to pressure waves reflections on walls and on obstacles.

Flame front position



Overpressure evolution



## Summary & Perspectives

- LES approach for deflagration developed and implemented in CALIF<sup>3</sup>S-P<sup>2</sup>REMICS software.
- Simulation of an accelerated deflagration with LES and RANS approaches:
  - ➡ Good agreement between LES numerical results and experimental data;
  - ➡ Dynamical formulation of the wrinkling factor necessary for a good reproduction of the flame front propagation;
  - ➡ RANS: dispersion of numerical results depending on the turbulent flame speed correlation used.
- Next step
  - ➡ Use LES approach (turbulent characteristics of the flow) in order to perform in indepth the interpretation of experiments and to support RANS model validation.
  - ➡ LES approach more predictive than RANS approach but too expensive for industrial purpose:
    - 2D simulations: 13 hours on 180 processors ( $6.5 \times 10^5$  cells,  $2.6 \times 10^5$  time steps),
    - 3D simulations: 20 days on 2500 processors ( $160 \times 10^6$  cells,  $2.6 \times 10^5$  time steps),
  - Development of an "hybrid" RANS/LES approach?