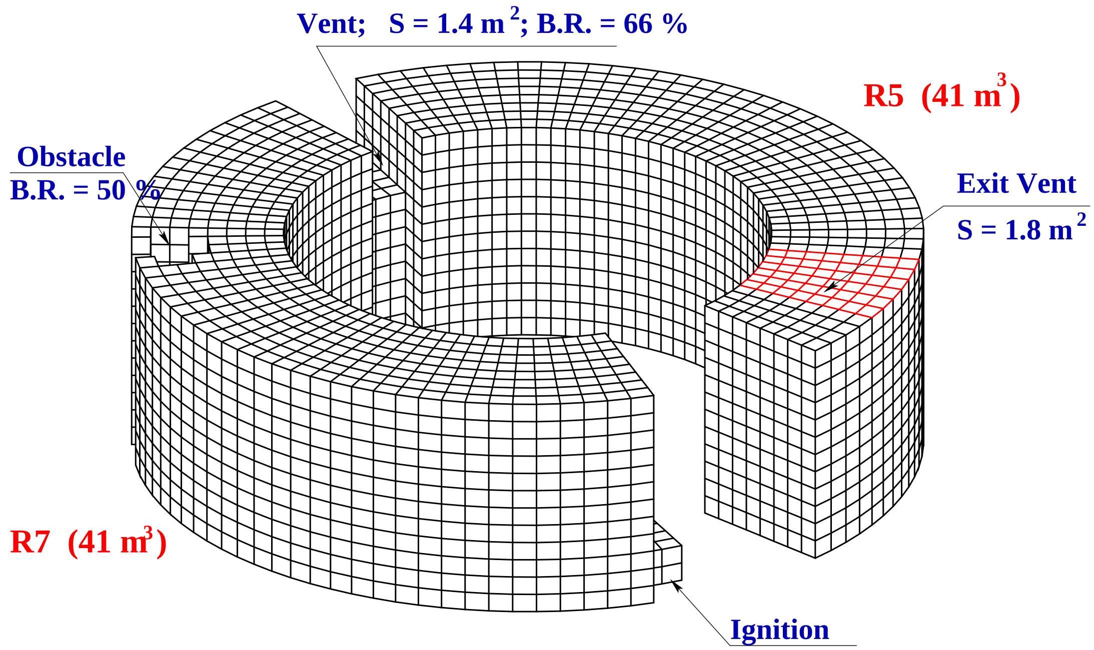
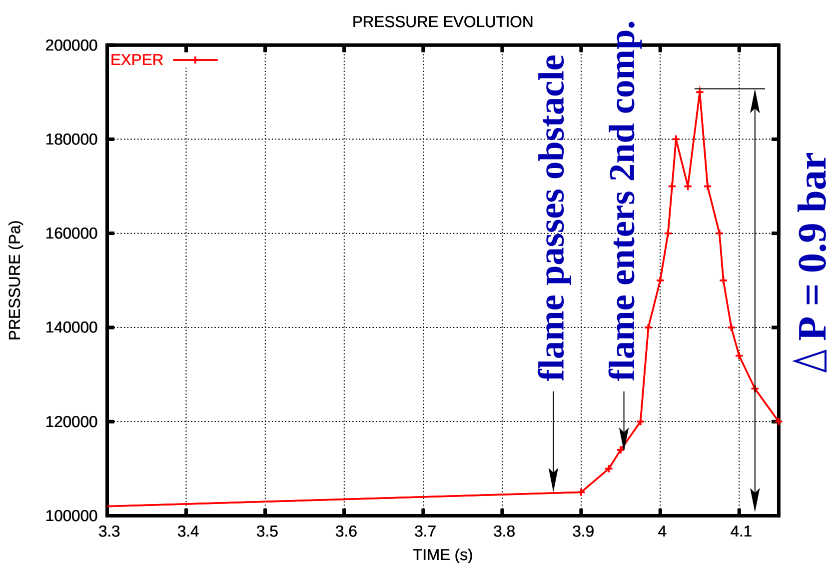
Club CASTEM 2004 November 26, 2004.

Simulation of HDR and BMC Hydrogen Combustion Tests with the TONUS code and CREBCOM model.

Hydrogen Deflagration Test Ex29 (BMC).

Initial conditions: 10 % H_2, P = 1 bar, T = 337 K.





Governing Equations.
CREBCOM combustion model.

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}) = 0 \quad (1)$$

$$\frac{\partial\rho Y_k}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}Y_k) = \rho\dot{\omega}_k \quad (2)$$

$$\frac{\partial\rho\vec{u}}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u}+P\mathbf{I}) = \rho\vec{g} \quad (3)$$

$$\frac{\partial\rho e_t}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}h_t) = \rho\vec{g}\cdot\vec{u} - \rho\sum_j h_j^0\dot{\omega}_j - H(T-T_0) \quad (4)$$

$$\frac{\partial\rho K_0}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}K_0) = 0 \quad (5)$$

$$\frac{\partial\rho Y_{H_2,f}}{\partial t} + \vec{\nabla}\cdot\left(\rho\vec{u}Y_{H_2,f}\right) = 0 \quad (6)$$

$$\frac{\partial\rho Y_{H_2,i}}{\partial t} + \vec{\nabla}\cdot(\rho\vec{u}Y_{H_2,i}) = 0 \quad (7)$$

Where

$$H_2 + \frac{1}{2}O_2 \longrightarrow H_2O$$

$$\xi = \frac{Y_{H_2} - Y_{H_2,i}}{Y_{H_2,f} - Y_{H_2,i}}$$

$$\dot{\omega}_\xi = \frac{K_0}{\triangle x} \times \{criter.function\}$$

“Automatic” Determination of the parameter K_0

METHOD (I) Source: A.A. Efimenko and S.Dorofeev. CREBCOM code system for description of gaseous combustion (2001).

$$\mathbf{K_0 = \frac{\sigma+1}{4} S_T = \frac{S_T}{S_L} \times \frac{\sigma+1}{4} S_L} \qquad (8)$$

Where

$$\begin{aligned}
\frac{S_T}{S_L} &= 0.5(\sigma-1)\left(\frac{L}{\delta}\right)^{1/3} Le^{-2/3} \quad if \quad \frac{L}{\delta} > 500 \\
\frac{S_T}{S_L} &= 0.0008(\sigma-1)^3\left(\frac{L}{\delta}\right) \quad if \quad \frac{L}{\delta} < 500 \\
L &= L_c \times max(0.1; 0.5(1-\sqrt{1-BR}))
\end{aligned}$$

METHOD (II) Source: S.Dorofeev and R. Redlinger. Description of FLAME3D (2003).

$$\mathbf{K_0 = \frac{\sigma+3}{8} S_T = \frac{S_T}{S_L} \times \frac{\sigma+3}{8} S_L} \qquad (9)$$

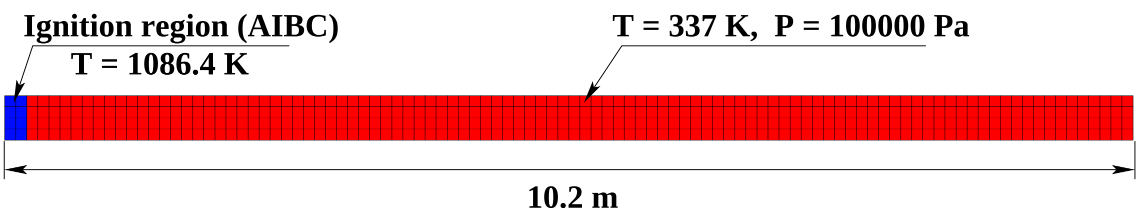
where

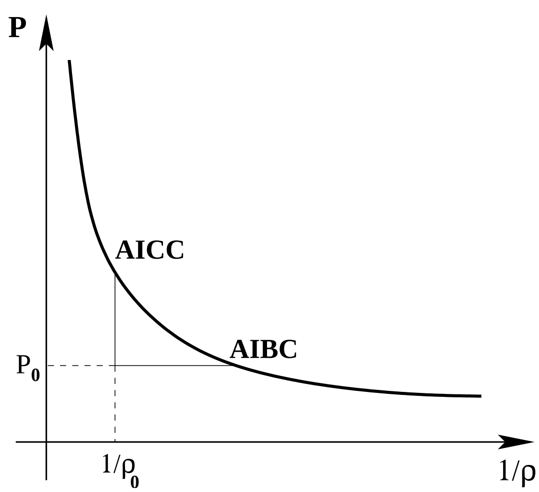
$$\frac{S_T}{S_L} \approx 30.0 \quad \textbf{for} \quad V/S/dx \approx 6.0$$

METHOD (III) Source: P. Pailhories. Bilan des calculs de combustion multi-D réalisés avec le modèle CREBCOM du code TONUS (2003).

$$\mathbf{K_0 = 66.7 \times S_L} \qquad for \qquad V/S/dx \approx 2.0 \qquad (10)$$

Presentation of the Ignition Problem

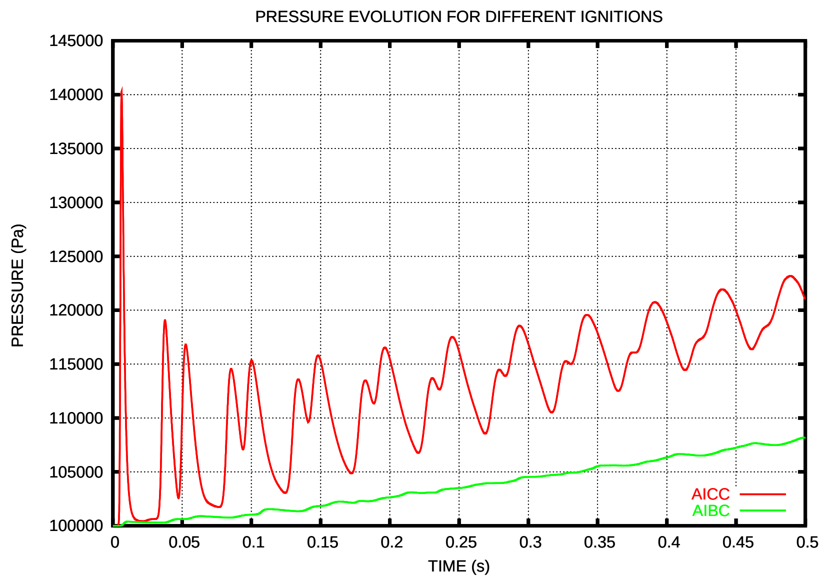


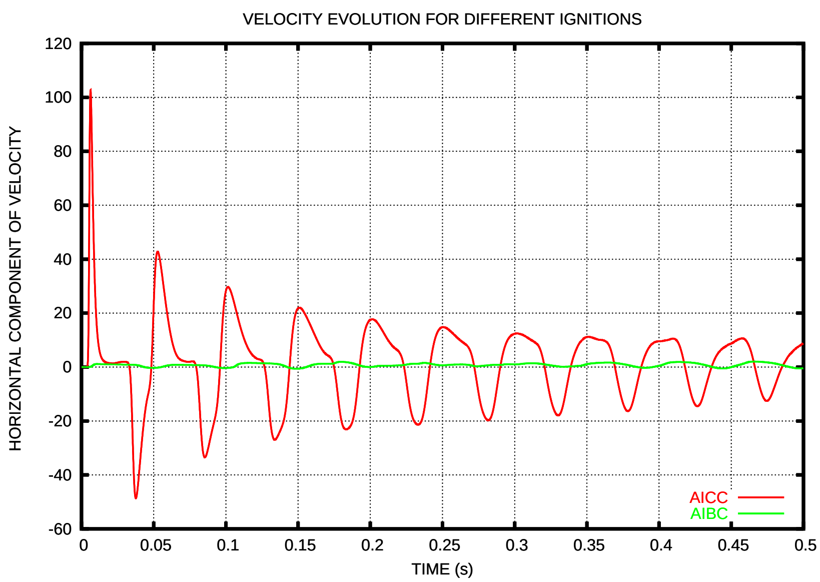


Two ways of ignition:

- **AICC** (Adiabatic Isochore Complete Combustion) $\rho_2 = \rho_1$;
  ($T \approx 1300$ K, $P \approx 3.65 \times 10^5$ Pa).
- **AIBC** (Adiabatic IsoBare complete Combustion) $P_2 = P_1$.
  ($T \approx 1086$ K).

Pressure and velocity evolution at the capteur



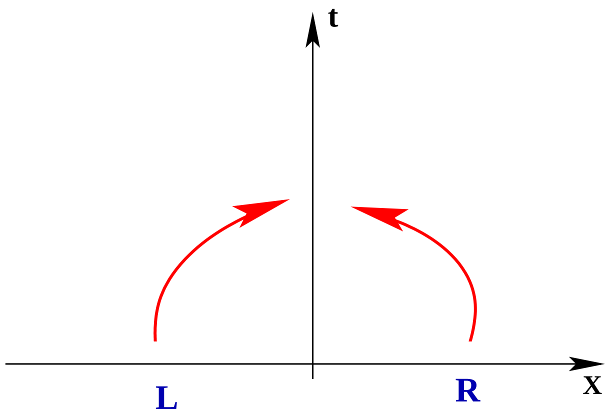


Choice of the Numerical Scheme (1)

a) **F**lux **V**ector **S**plitting scheme (VLH)

$$\mathbf{F}_{num}(\mathbf{U}_L, \mathbf{U}_R) = \mathbf{F}^+(\mathbf{U}_L) + \mathbf{F}^-(\mathbf{U}_R) \qquad (11)$$

Stationary contact line is diffused.



b) **F**lux **D**ifference **S**plitting scheme (SS)

$$\mathbf{F}_{num}(\mathbf{U}_L, \mathbf{U}_R) = \mathbf{F}(RP(0; \mathbf{U}_L, \mathbf{U}_R) \qquad (12)$$

Stationary contact line is resolved.

Choice of the Numerical Scheme (2)

1D results.

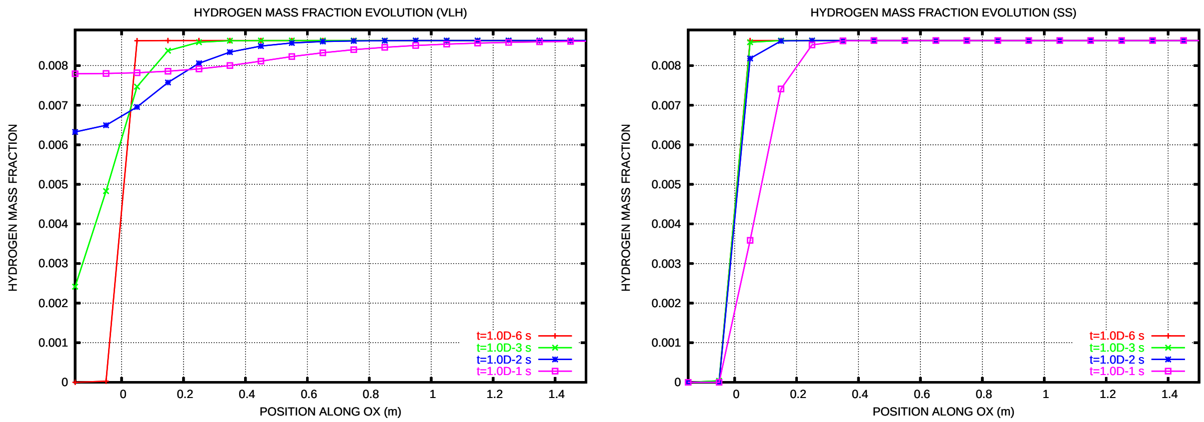


Figure 1: **Hydrogen Mass Fraction Evolution using VLH scheme (left) and SS scheme (right)**

2D results.

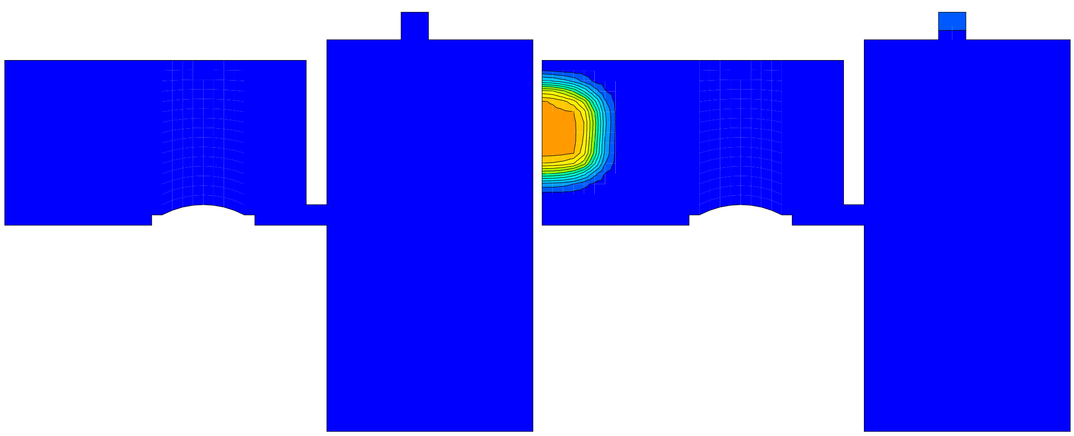
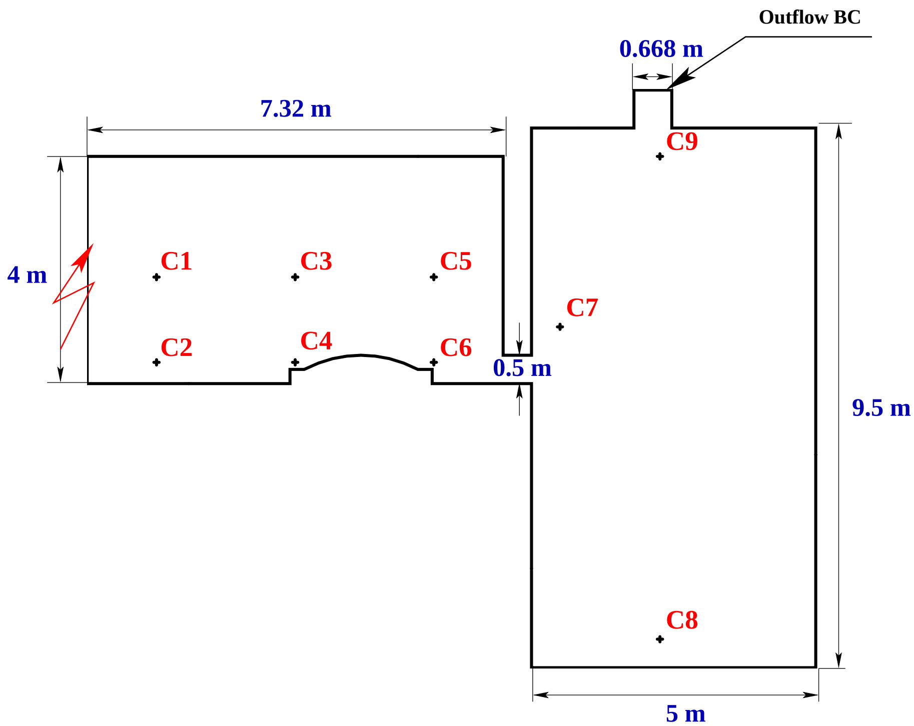


Figure 2: **Temperature isolines at** $t = 1.0$ **s using VLH(2nd order) scheme (left) and SS(2nd order) scheme (right).** $\triangle T$ **between isolines is** 62.75 **K.**

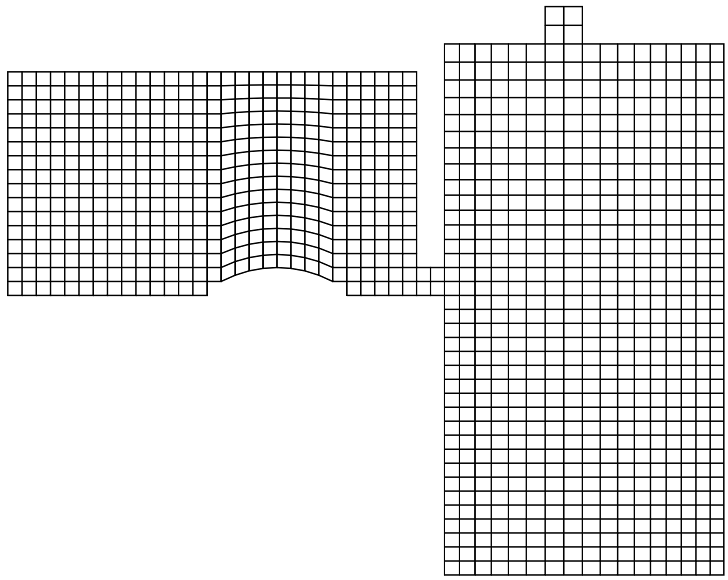
E12.3.2 computation using 2D geometry.

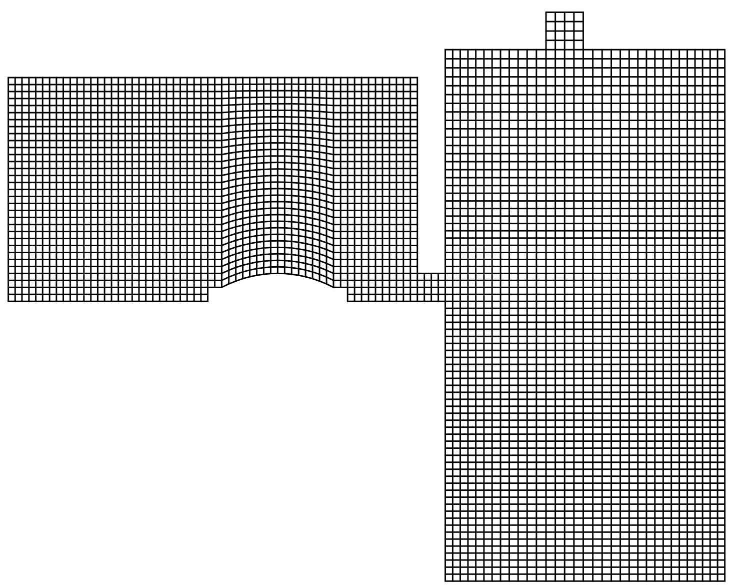


Method	R1904	R1905	R1801
I	7.48	7.48	11.08
II	9.38	9.38	9.38
III	18.9	18.9	18.9
2D, present comp.	0.41	0.41	3.7
3D, present comp.	0.55	0.55	2.8

Table 1: **HDR Test E12.3.2**. Values of K_0 computed using different methods.

E12.3.2 computation. Mesh of 1074 and 4256 elements

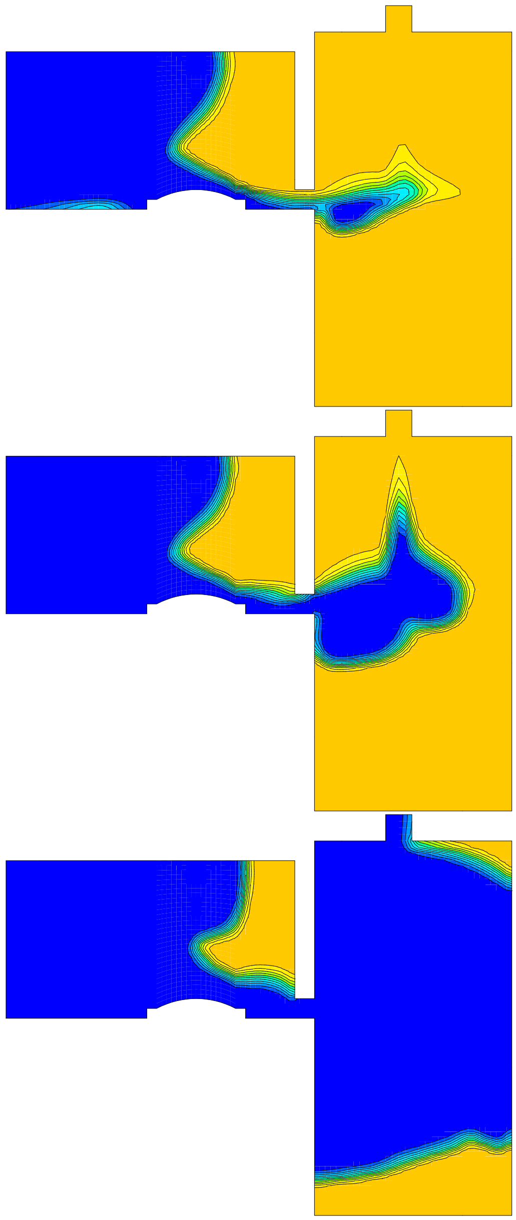




2D version of the E12.3.2 computation.

Hydrogen Mass Fraction Evolution. Fine Mesh.

$t = 2.4$ **s,** $t = 2.5$ **s and** $t = 2.9$ **s**



Pressure evolutions. Effect of the Grid Refinement.

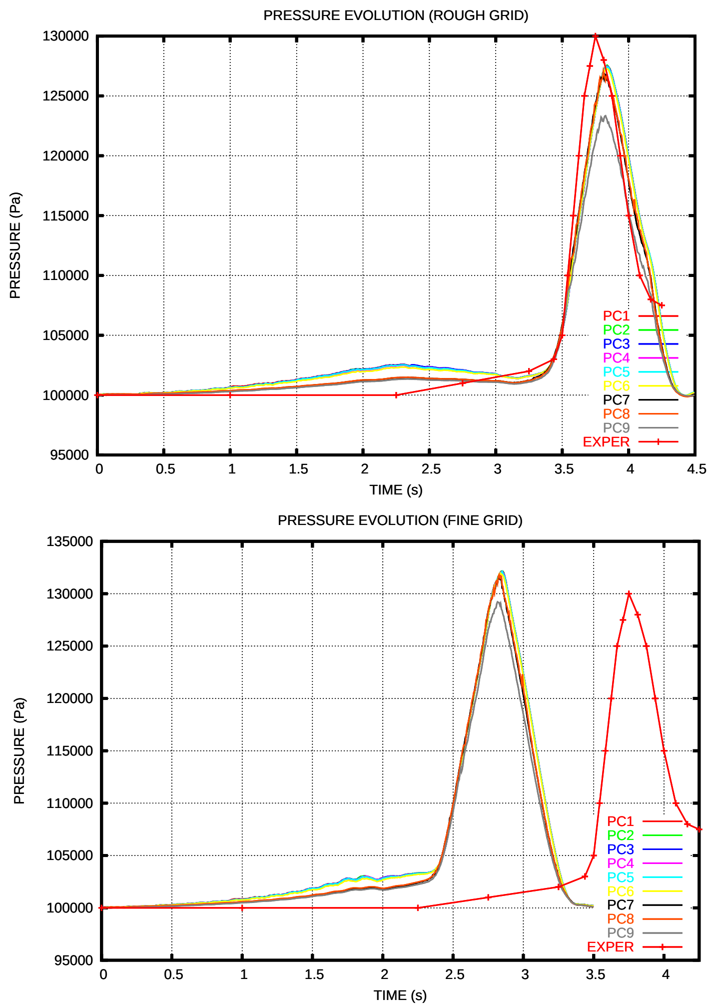
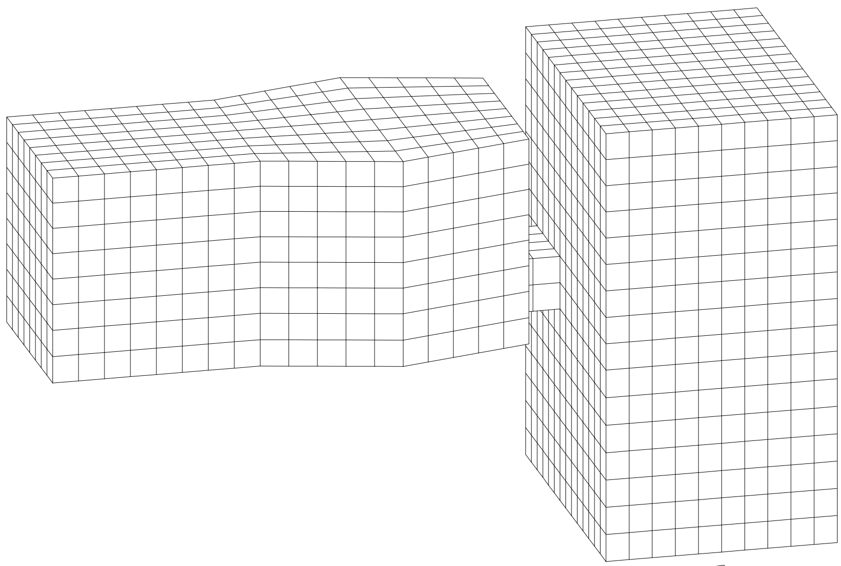


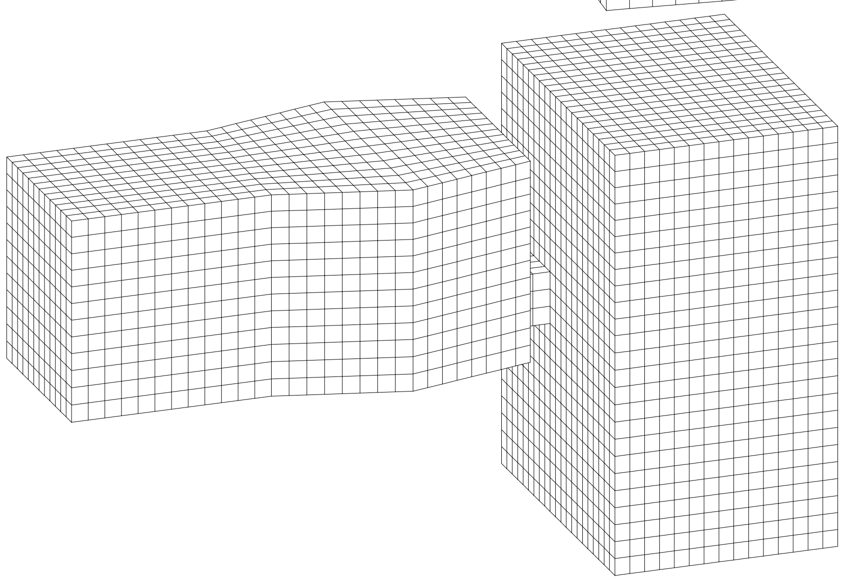
Figure 3: **HDR test E12.3.2 in 2D geometry.** Pressure histories corresponding to the coarse mesh (top) and the fine mesh (bottom). **The red line corresponds to the experimental results.**

3D version of the E12.3.2 computation.

Mesh of 3 412 elements ($\triangle x \approx 0.55$ m) (top)

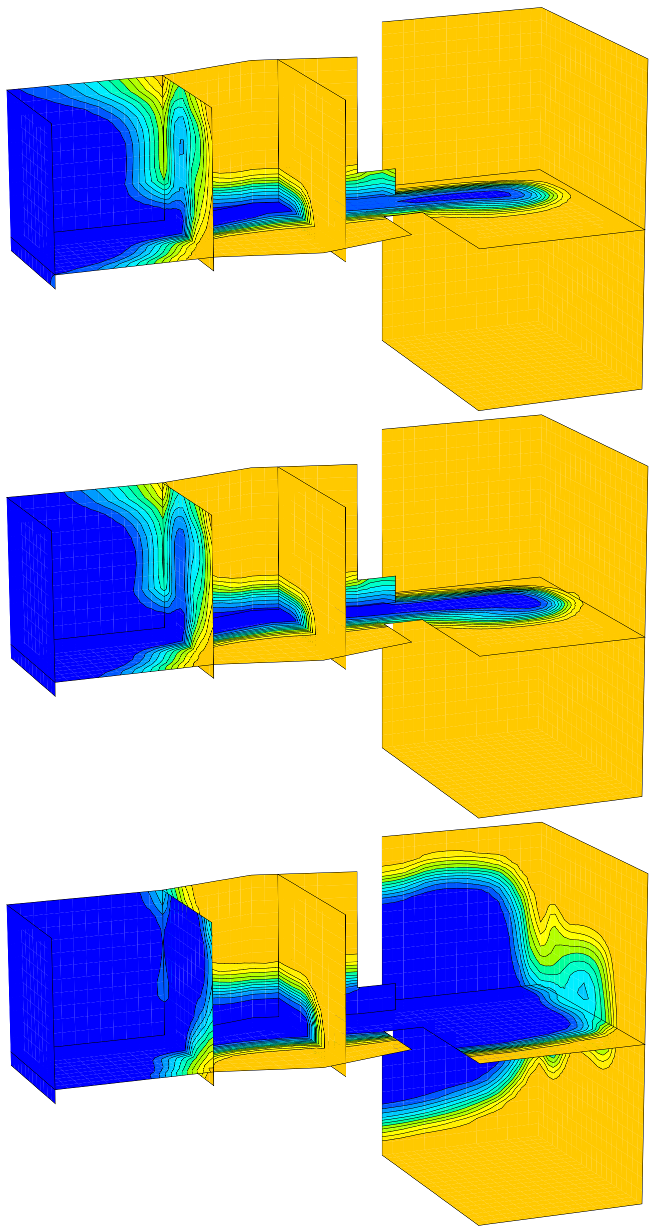
Mesh of 11 965 elements ($\triangle x \approx 0.37$ m) (bottom)





3D. Hydrogen Mass Fraction Evolution. Fine Mesh.

$t = 2.4$ **s,** $t = 2.5$ **s and** $t = 2.9$ **s**



3D. Pressure evolutions. Effect of the Grid Refinement.

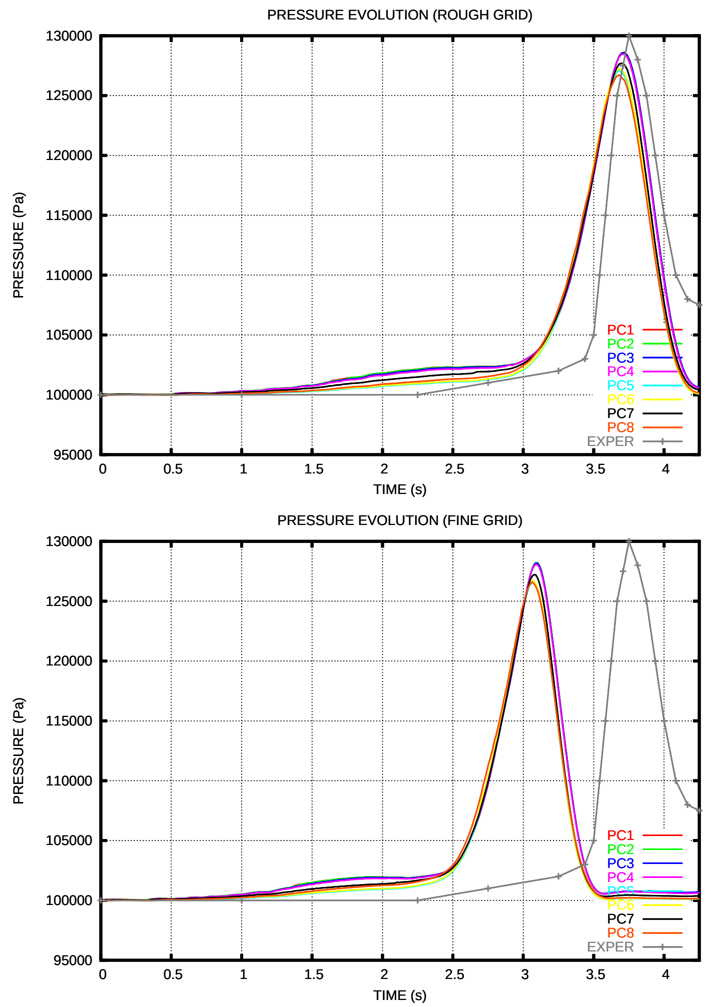


Figure 4: **HDR test E12.3.2 in 3D geometry**. Pressure histories corresponding to the coarse mesh (top) and the fine mesh (bottom). **The grey line corresponds to the experimental results.**

Hydrogen Deflagration Test Ex29.

Method	R7a	R7b	R5
I	12.86	13.04	18.13
II	11.4	11.4	11.4
III	33.6	33.6	33.6
3D, present comp.	0.265	25.0	20.0

Table 2: **BMC Test Ex29**. Values of K_0 obtained using different methods.

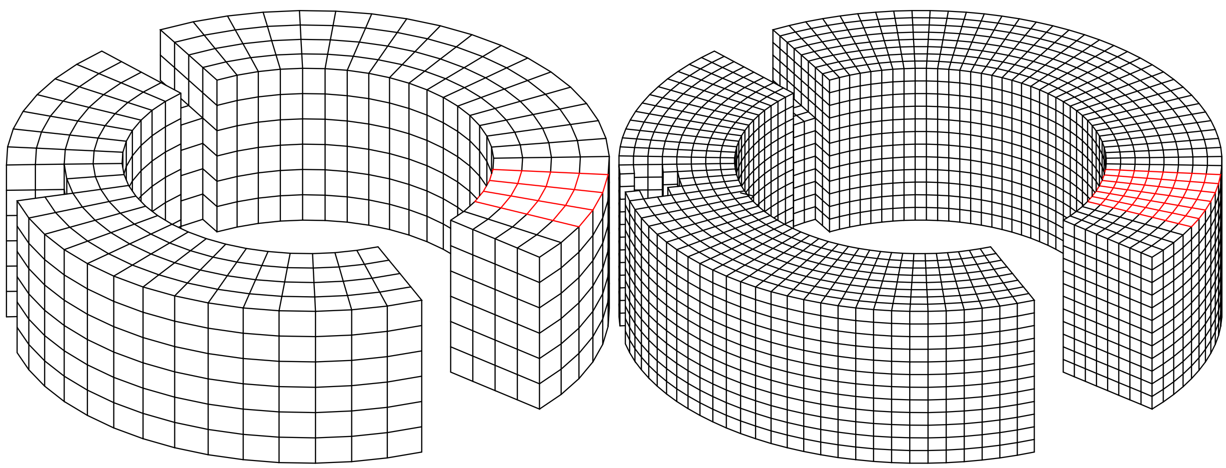
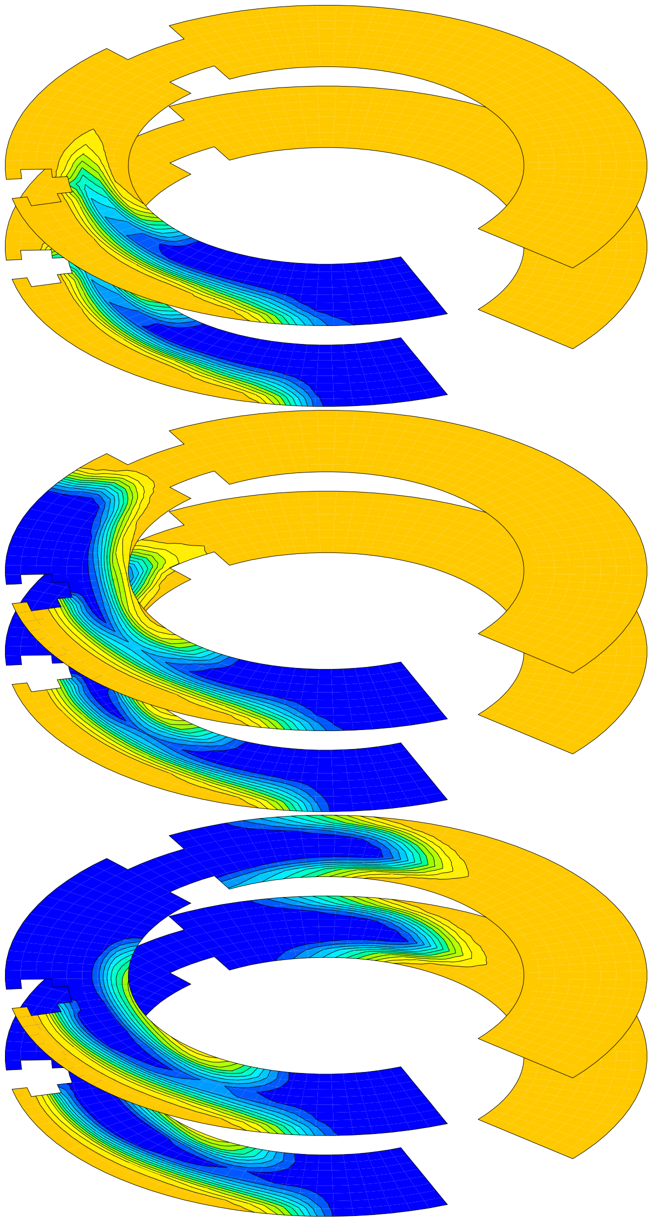


Figure 5: **BMC test Ex29 in 3D geometry**. Grid of 1098 elements (left; $\triangle x_{ave} = 0.41526$ m) and grid of 8832 elements (right; $\triangle x_{ave} = 0.2078$ m)

Hydrogen Deflagration Test Ex29.

Hydrogen Mass Fraction Isolines at

$t = 2.875$ **s,** $t = 2.925$ **s and** $t = 2.95$ **s**



Hydrogen Deflagration Test Ex29.
Comparison with Experimental Results.

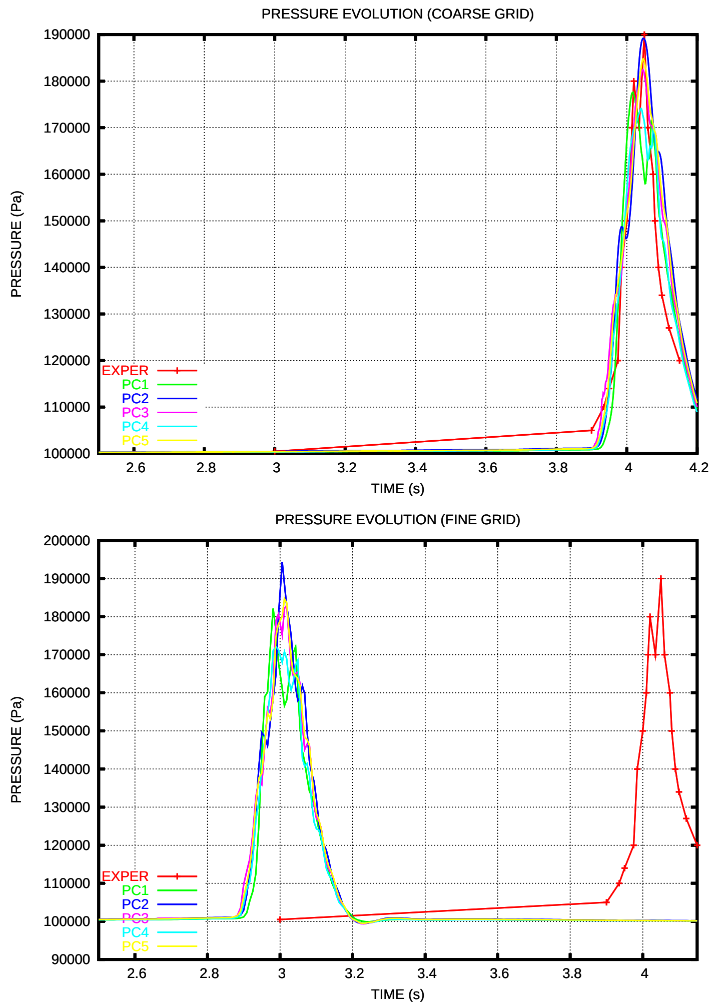


Figure 6: **BMC test Ex29 in 3D geometry**. Pressure histories corresponding the coarse mesh (left) and the fine mesh (right). **The red line corresponds to the experimental results.**