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Thermodynamic Aspects of Interaction Between Premixed Hydrogen Flame and Water Droplets

GAI Guodong
Sergey KUDRIAKOV

DEN/DANS/DM2S/STMF/LATF

Saclay, France

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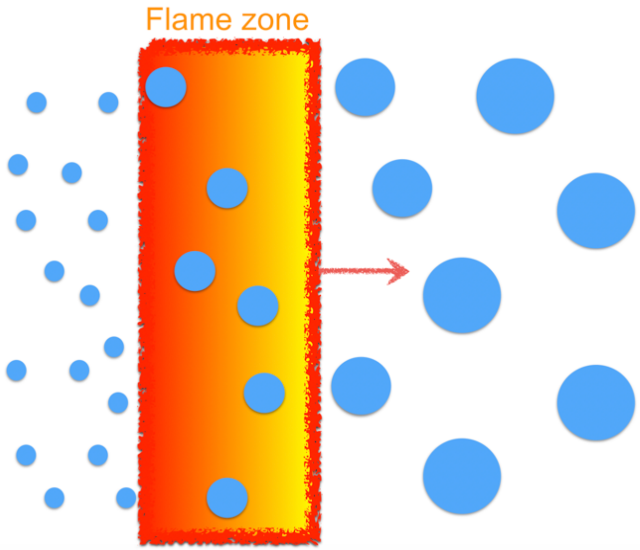
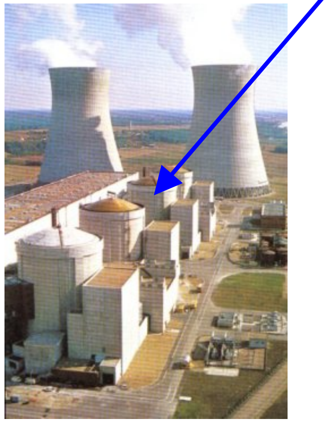
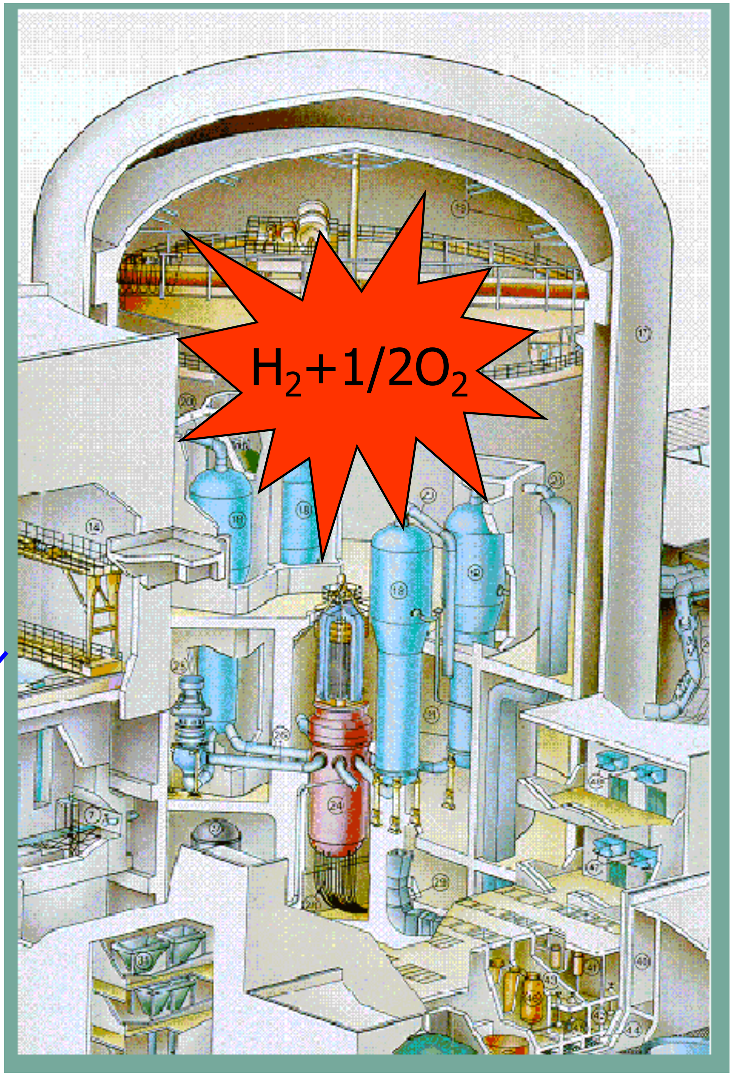
Introduction

- ✓ The course of a serious accident
- ✓ Spray system of the PWR
- ✓ Interaction between flame and spray



THE COURSE OF A SEVERE ACCIDENT





Severe accidents

$Zr+2H_2O=>ZrO_2+2H_2$

rejection of H_2

Formation of a mixture potentially explosive
$H_2 + H_2O + Air$

sources of ignition

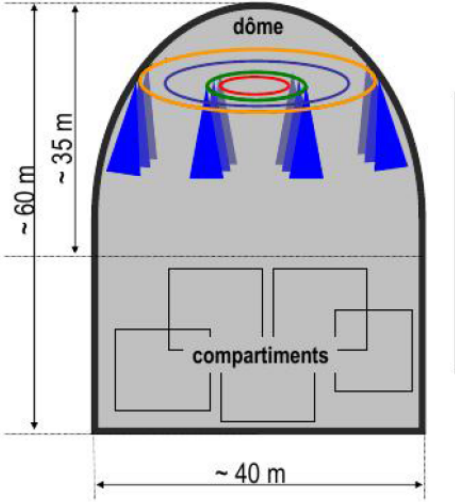
Propagation of flames:
(Rapid deflagration or .... detonation)

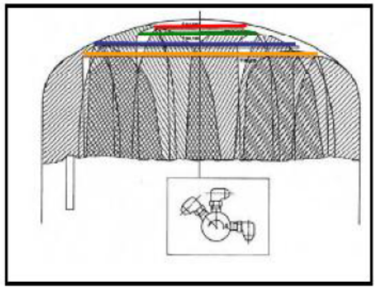
Pressure loads →
Threat to the containment

We must estimate the consequences of an hydrogen explosion !!!

SPRAY SYSTEM OF THE PWR

Spray system (PWR 900 MWe)





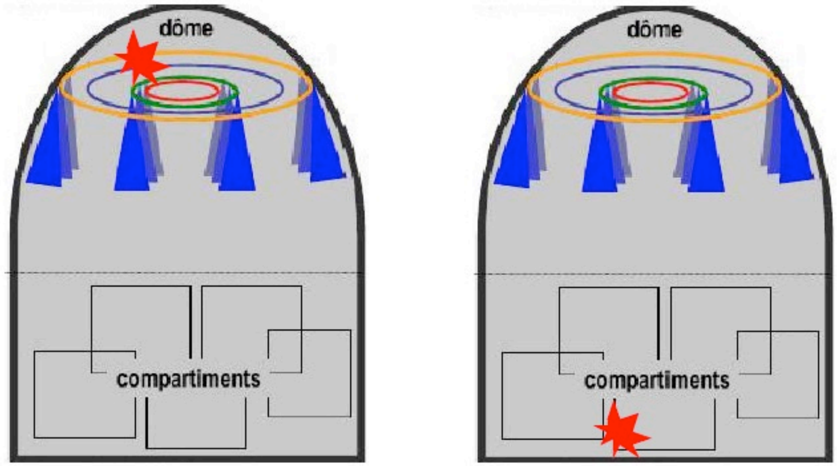
$D_{32} {\sim} 500 \mu m$

<u>In order to:</u>

- *Limit the pressure*
  inside the containment via steam condensation
- *Capture the fission products*
  to prevent radioactive release
- *Mix gaseous species*

<u>Source: [Foissac 2011]</u>

The mixture can be ignited <u>during</u> the spray phase!!!



<u>The action of spray can lead to:</u>

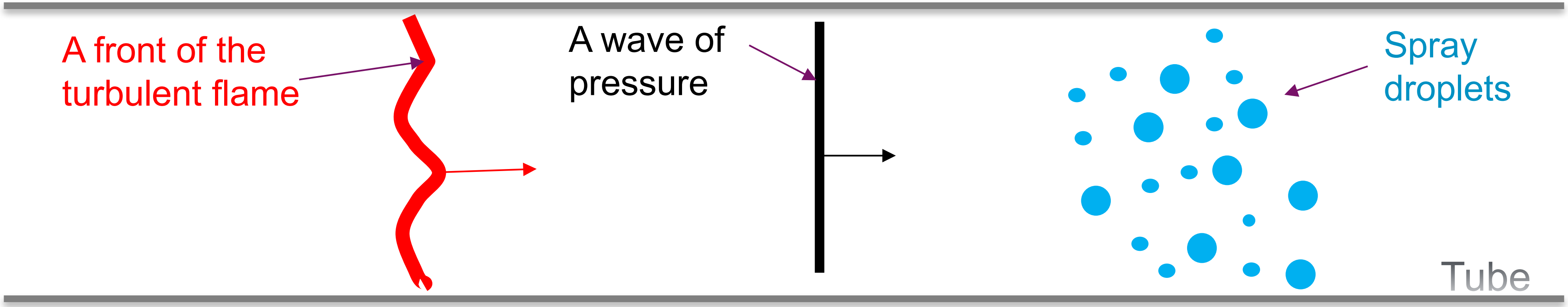
1. Overpressure Mitigation

or, on the contrary,

2. Flame Acceleration

<u>Source: [Wingerden 1995], [Gupta, 2014]</u>

PHENOMENA

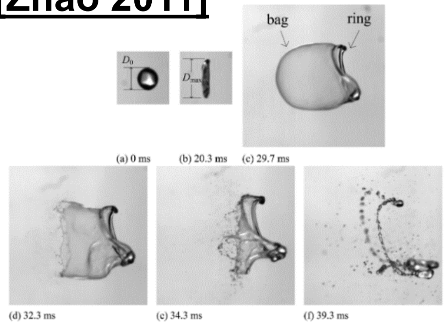

A front of the turbulent flame

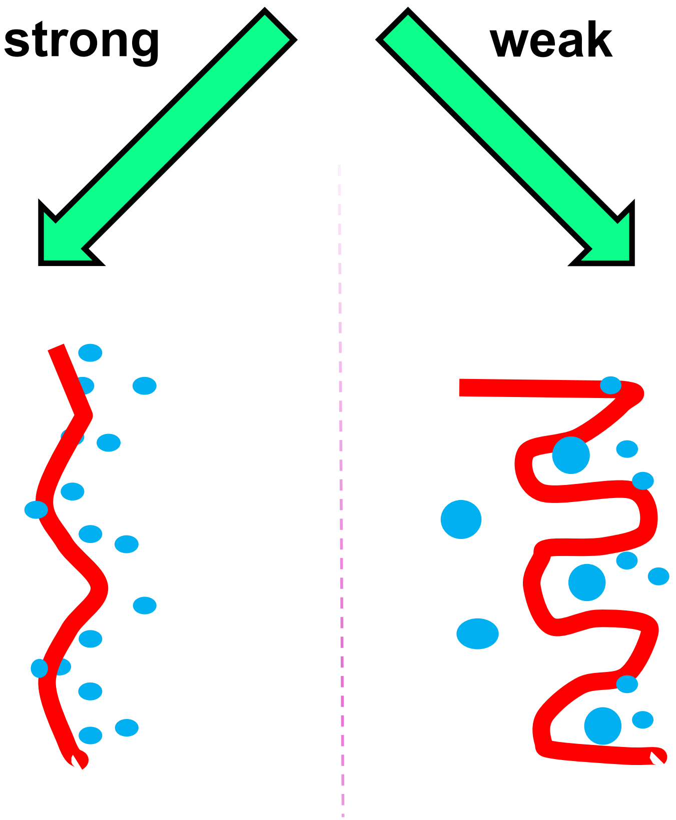
A wave of pressure

Spray droplets

Tube

Source: [Zhao 2011]




strong

weak

- Break-up of the water droplets
- Dilution of flame with the fin droplets

The velocity of the flame is reduced.

- Increase the flame surface *S*
- Interaction flame-turbulence

The velocity of the flame increases.

OBJECTIVES

- Investigation on ***Thermodynamic*** aspects of the interaction flame-spray, behind the flame front, with the ***Lumped-parameter*** and ***CFD model***

- Analysis of real ***Experimental*** works by applying the ***CREBCOM model*** with ***Evaporation*** process

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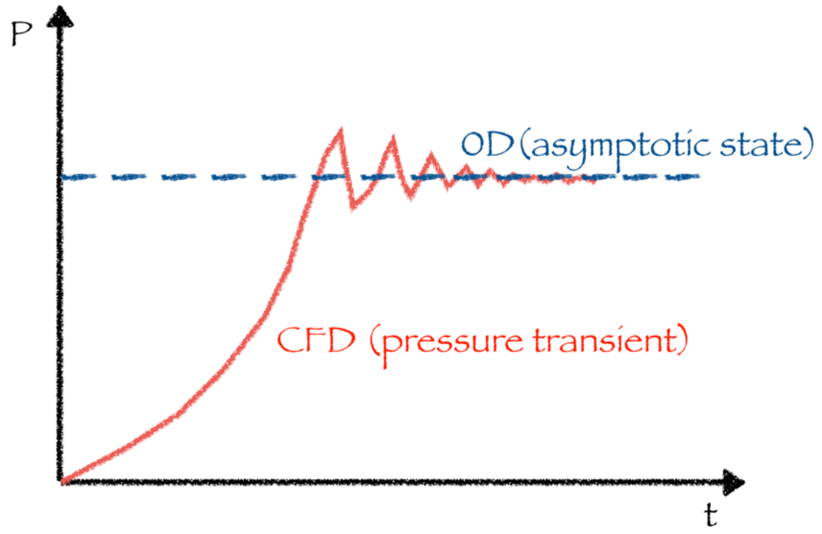
Lumped-parameter Approach

- ✓ Main hypothesis and definitions
- ✓ Governing equations
- ✓ Test cases



MAIN HYPOTHESIS AND DEFINITIONS

Fresh gas

Liquid water

Complete Combustion

Total Evaporation

Burnt gas

- ***Ideal*** gas mixture
- One irreversible chemical reaction
  $H_2 + ½O_2 \rightarrow H_2O$
- T_{ini} *and* P_{ini} constant, m_0 change with X_{H_2}
- The system is ***closed*** and ***adiabatic***

Volume fraction of liquide phase: $\alpha = \frac{V_{liq}}{V_{tot}}$

Conservation of mass:

$$\tilde{m}_0 = \tilde{m}_f \quad \tilde{m}_f = \sum_{j=1}^{4} n_j^{fin} M_j + m_{H_2O}^{liq\rightarrow vap}$$

Conservation of energy:

$$\tilde{e}_0 = \tilde{e}_f$$

$$\tilde{e}_0 = \sum_i Y_i^{ini} h_i^0 + \int_0^{T_0} \left\{ \sum_i Y_i^{ini} c_{v,i}(T') \right\} dT' + Y_{H_2O}^{liq} u_{H_2O}^{liq}$$

SEVERAL CASES CONSIDERED

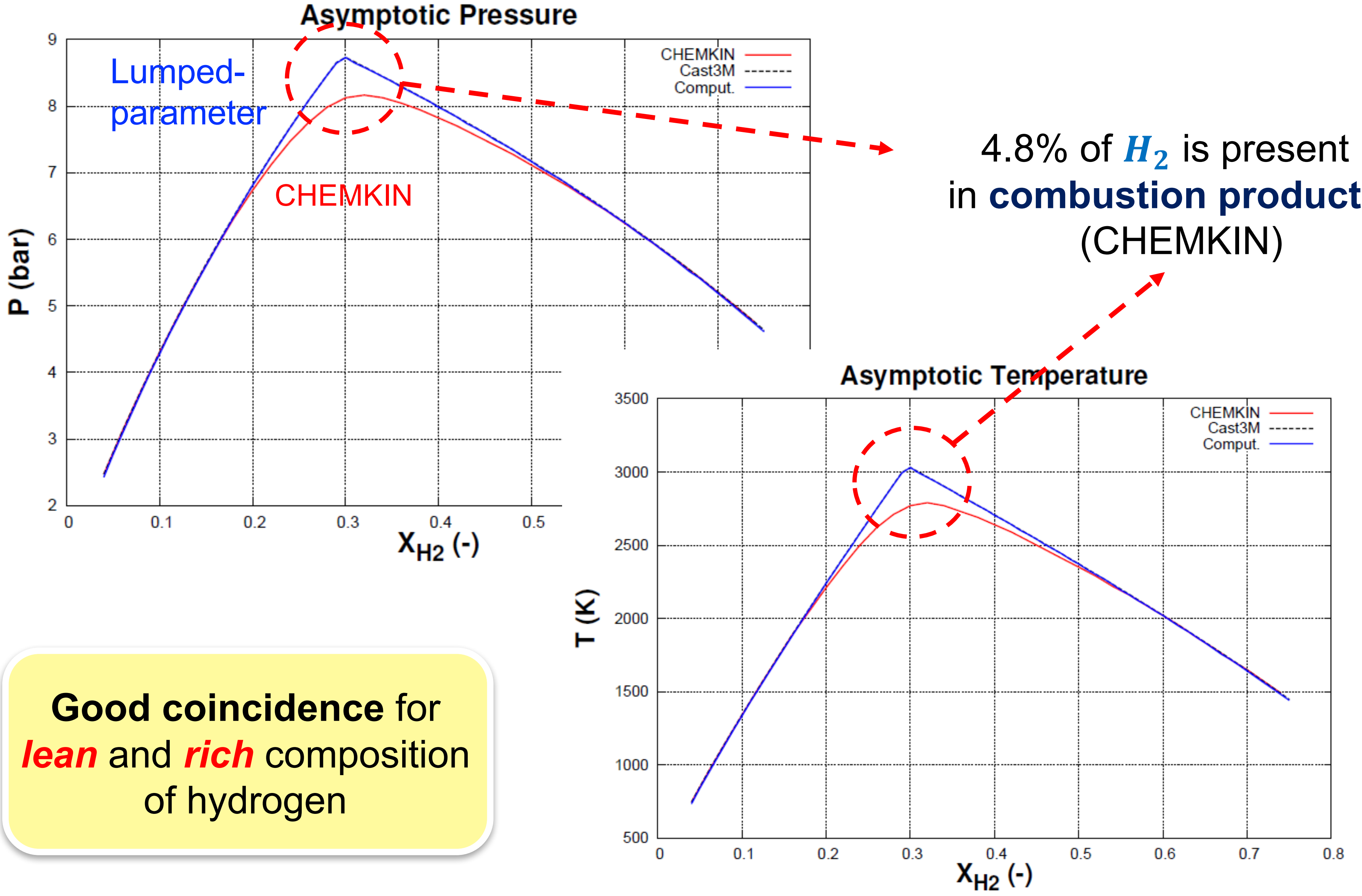
Case	P_{ini} (bar)	T_{ini}^{gas} (K)	T_{ini}^{liq} (K)	$X_{H_2}^{ini}$(-)	$X_{H_2O}^{vap,ini}$(-)	α (-)
I	1.0134	300.0	-	$[0.04, 0.75]$	0.0	0.0
II	1.0134	300.0	298.15	$[0.04, 0.75]$	0.0	$[0.0, 2.0 \times 10^{-3}]$
III	1.0134	293.15	293.15	$[0.04, 0.75]$	0.0	$(2.0, 3.0, 4.0) \times 10^{-4}$
IV	2.4	393.15	293.15	$[0.09, 0.30]$	0.45	$(2.0, 3.0, 4.0) \times 10^{-4}$

Table: Initial conditions for different cases

- ☐ Case I: Comparison with CHEMKIN code
- ☐ Case II: Limiting liquid volume fraction (α_{lim})
- ☐ Case III: Influence of liquid volume fraction (α)
- ☐ Case IV: « Accidental » initial conditions*

Source: [Malet 2008]

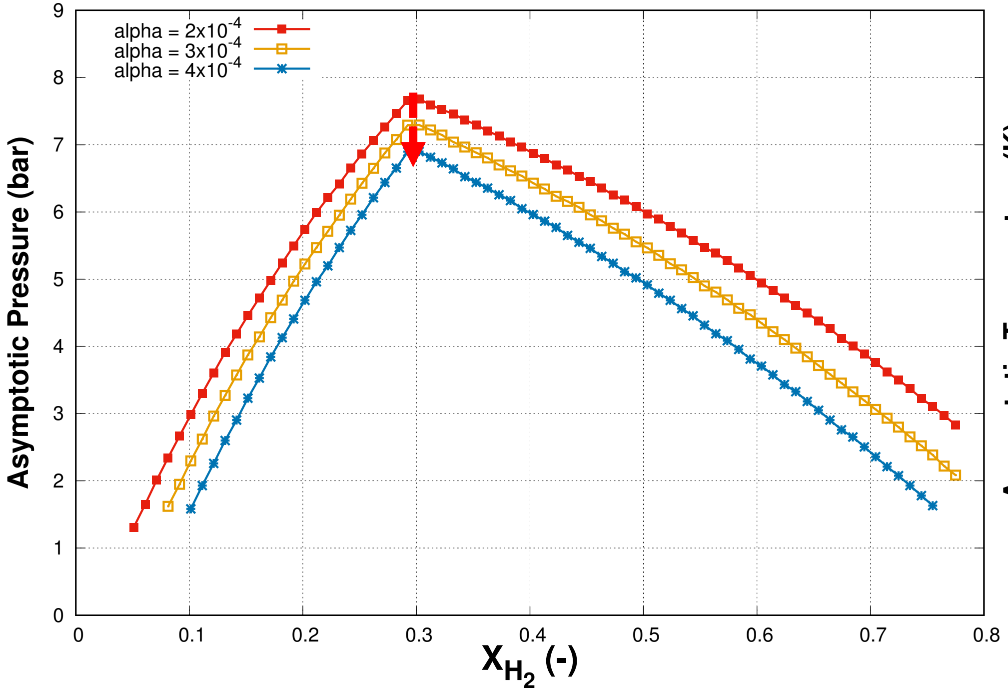
CASE I: COMPARISON WITH CHEMKIN

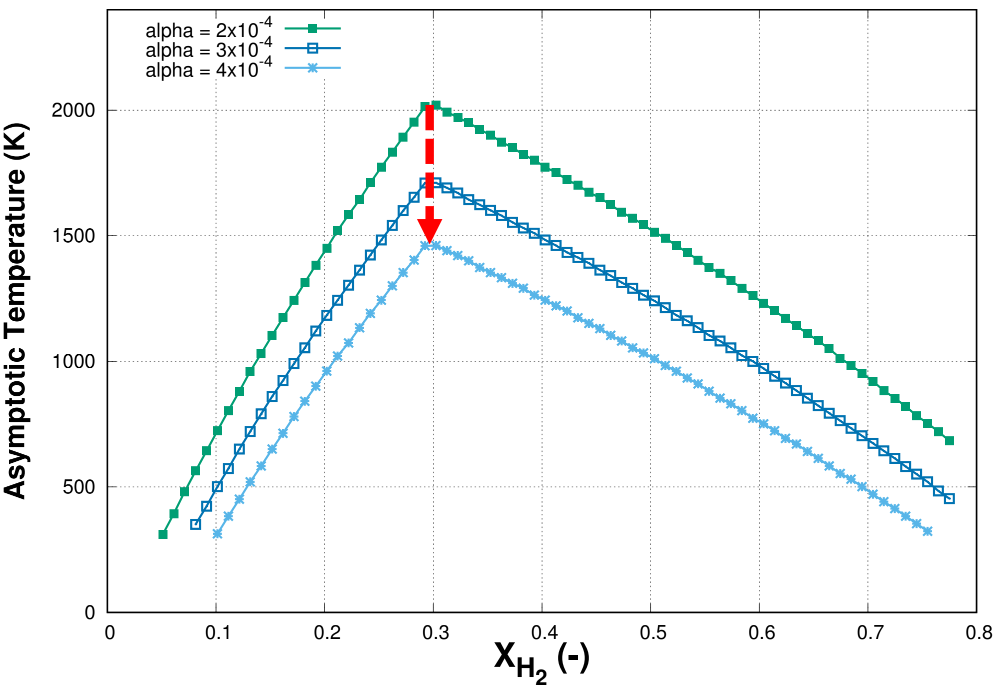


4.8% of H_2 is present
in **combustion products**
(CHEMKIN)

Good coincidence for
lean and ***rich*** composition
of hydrogen

CASE III: INFLUENCE OF LIQUID FRACTION





	$T_{max}(K)$	$P^*_{max}(\text{bar})$
$\alpha = 0$	3022	8.72
$\alpha = 2\times10^{-4}$	2000	7.68
$\alpha = 3\times10^{-4}$	1710	7.29
$\alpha = 4\times10^{-4}$	1460	6.9

*Pressure for ***stoichiometric*** initial hydrogen-air mixture

Mitigation of the flame
Effective
depressurization effect

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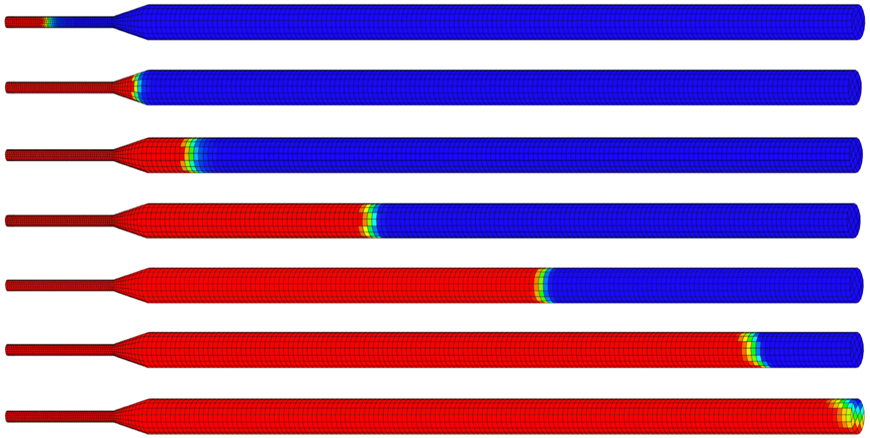
CREBCOM CFD model

- ✓ Numerical model and main hypothesis
- ✓ Validation of the model and pressure transient
- ✓ Experimental investigation



NUMERICAL COMBUSTION MODEL

CREBCOM model:

Mass conservation: $$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u}) = 0$$

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

Momentum conservation: $$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u} + P\boldsymbol{I}) = \rho \vec{g}$$

Energy conservation: $$\frac{\partial \rho e_t}{\partial t} + \vec{\nabla} \cdot (\rho \vec{u} h_t) = \rho \vec{g} \cdot \vec{u} - \rho \sum_i \Delta h_{f,j} \dot{\omega}_j + S_{cr}$$

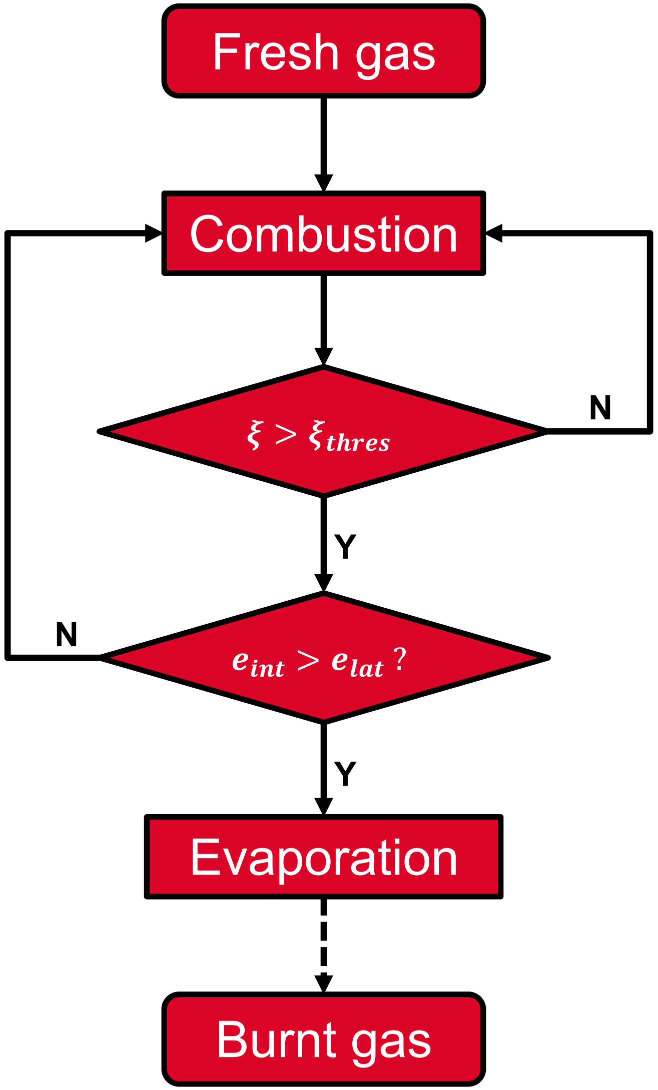
Combustion rate: $$\dot{\omega}_\xi = \frac{\boxed{K_0}}{\Delta x} \cdot \{criterion\ function\}$$

Thermal source term: $$S_{cr} = \boxed{-H}(T - T_0)$$

Progress variable: $$\xi(\vec{r}, t) = \frac{Y_{H_2}(\vec{r}, t) - Y_{H_2,ini}}{Y_{H_2,fin} - Y_{H_2,ini}} \qquad \begin{cases} \xi = 0 & \text{fresh gas} \\ \xi = 1 & \text{burnt gas} \end{cases}$$

Source: [Efimenko 2001]

MAIN HYPOTHESIS OF EVAPORATION



Fresh gas

Combustion

$\xi > \xi_{thres}$

N

Y

$e_{int} > e_{lat}$?

N

Y

Evaporation

Burnt gas

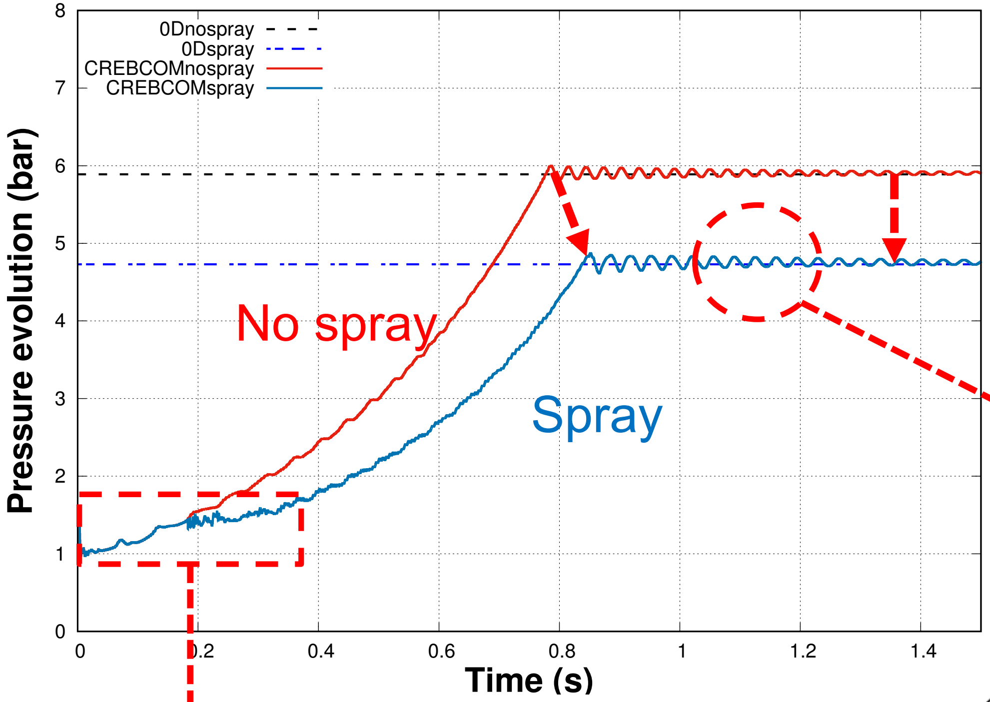
Preliminary assumptions:

- ○ Stationary droplets in fresh gas : $\vec{v}^{u}_{drop} = \mathbf{0}$
- ○ No interaction between droplets and fresh gas
- ○ Droplets evaporate ***totally*** and ***immediately*** across the flame if criteria satisfied
- ○ Evaporation takes place in a ***closed adiabatic*** cell

Criteria for evaporation:

1. $\xi(\vec{r},t) = \frac{Y_{H_2}(\vec{r},t) - Y_{H_2,ini}}{Y_{H_2,fin} - Y_{H_2,ini}} > \xi_{threshold}$
2. Sufficient volumetric internal energy for the complete evaporation of the liquid phase (heat-up of droplets and latent heat)

PRESSURE TRANSIENT



Volume fraction: $\boldsymbol{\alpha = 2\times10^{-4}}$

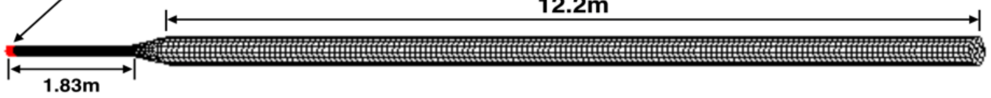
$\Delta t_{peak} \approx 0.1\ s$

$\Delta P_{peak} \approx 1.1\ bar$

Two main effects of ***evaporation***

Validation of the CREBCOM code

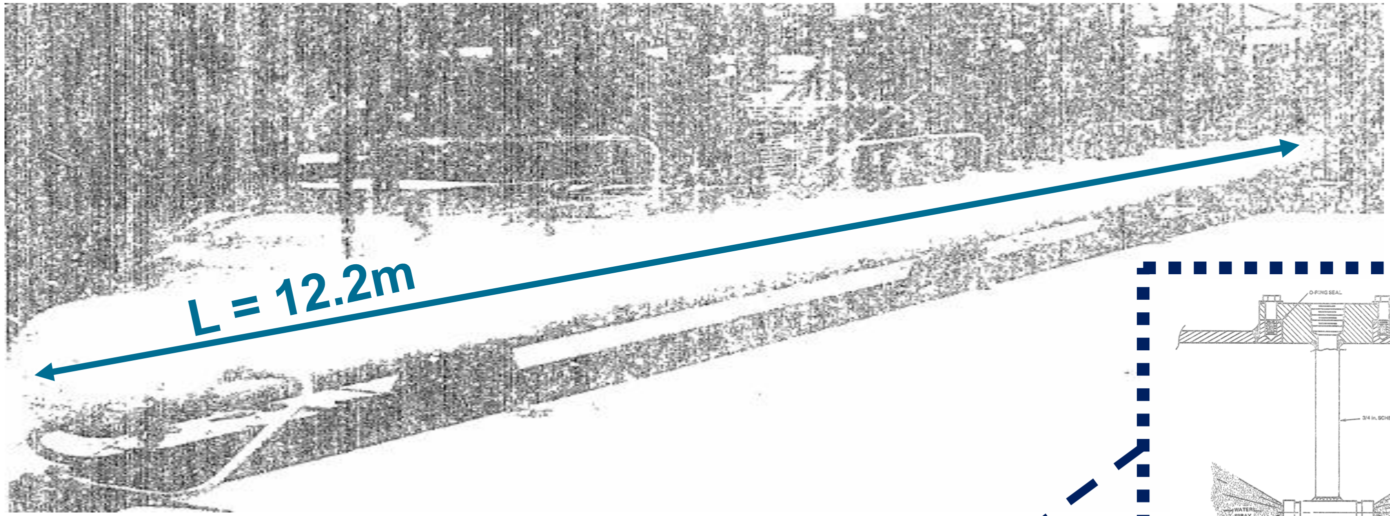
Good Coincidence



Second criteria of evaporation
No evaporation period

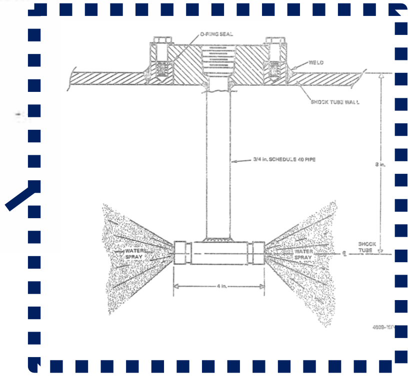
Deceleration of flame
Effective depressurization
Delay of peak pressure

EXPERIMENTAL FACILITY



$D = 0.406\ m$

Fig. Experimental **tube**



Opposite spray

Spray nozzle sketch

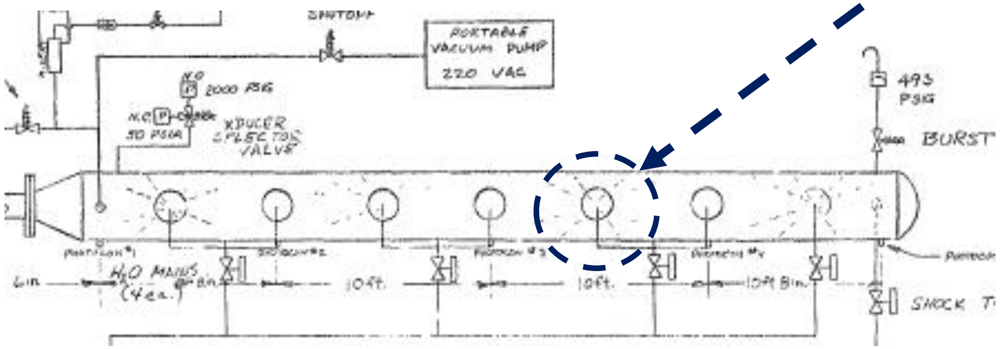
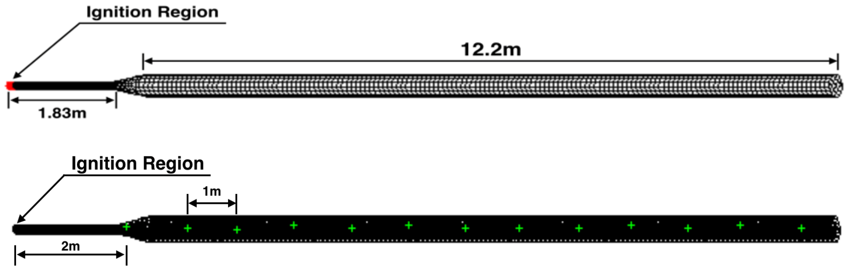


Fig. Arrangement of nozzles



Geometry used in the CREBCOM calculation

Source: [Carlson 1973]

EXPERIMENTAL RESULTS

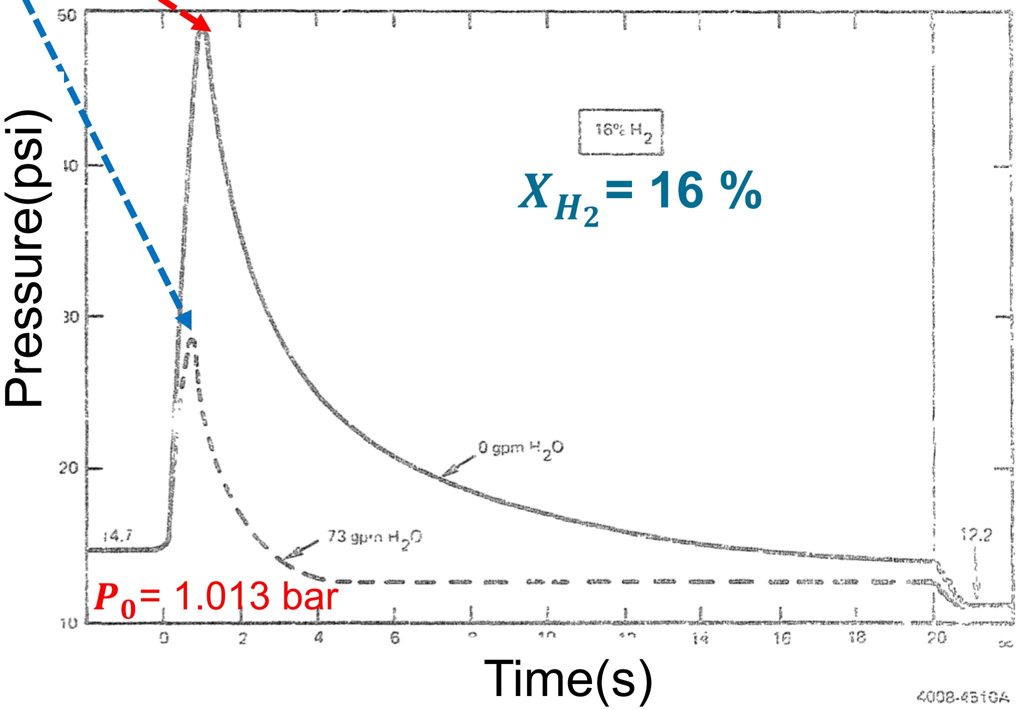
Fig. Important test cases

Test No.	X_{H_2} (dry)	Q_{spray} (l/s)	P_0 (atm)	P_{max} (atm)
4	12.0	0.0	1.0	1.97
5	12.0	4.7	1.0	1.36
7	16.0	0.0	1.0	3.32
8	16.0	4.6	1.0	1.94
10	12.0	0.0	1.5	3.67
11	12.0	4.5	1.5	2.7
12	16.0	0.0	1.5	4.76
13	16.0	4.5	1.5	3.13

Evaporation rate: $\dot{\alpha} = \frac{d\alpha}{dt}$

X_{H_2} = 16 % → P_{AICC^*} = 5.9 bar

Fig. Pressure transient evolution



*AICC = Adiabatic Isochoric Complete Combustion

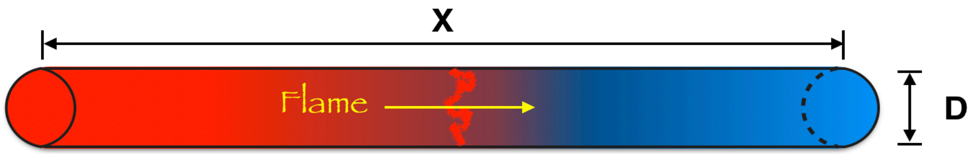
Source: [Carlson 1973]

Important **heat loss**

Mitigation **effect of spray**

Continuous spray and evaporation

FLAME VELOCITY DETERMINATION



Run-up distance:

X$_S$: position where the V_{flame} reaches C_{sp} in the *combustion products*

For $16\%H_2$, C_{sp}= 787 m/s

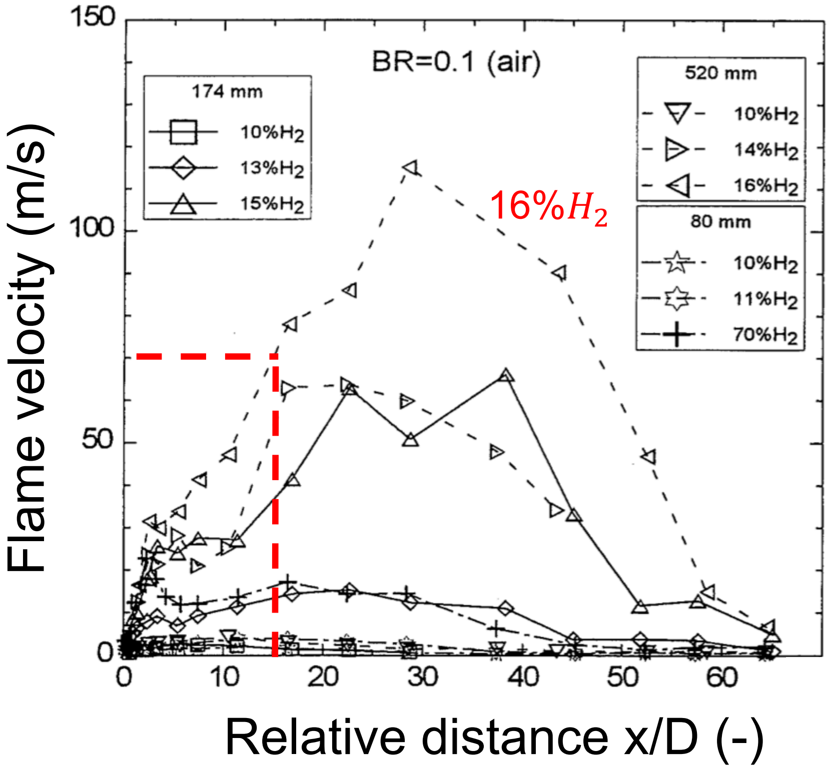
Source: [Dorofeev 2009]

$$\frac{X_S}{D} = \frac{\gamma}{C}\left(\frac{1}{\kappa} ln\left(\frac{\gamma D}{h}\right) + K\right) \qquad \gamma = \left(\frac{c_{sp}}{\mu^2(\sigma-1)^2 S_L}\left(\frac{\delta}{D}\right)^{\frac{1}{3}}\right)^{\frac{3}{6m+7}}$$

$$\frac{D}{h} = \frac{2}{1-\sqrt{1-BR}} \longrightarrow \frac{X_S}{D} \approx \mathbf{110} > \frac{L}{D} = \mathbf{30}$$

$$\longrightarrow \boldsymbol{v_{max} \ll C_{sp} = 787\ m/s}$$

Source: [Kuznetsov 1999]



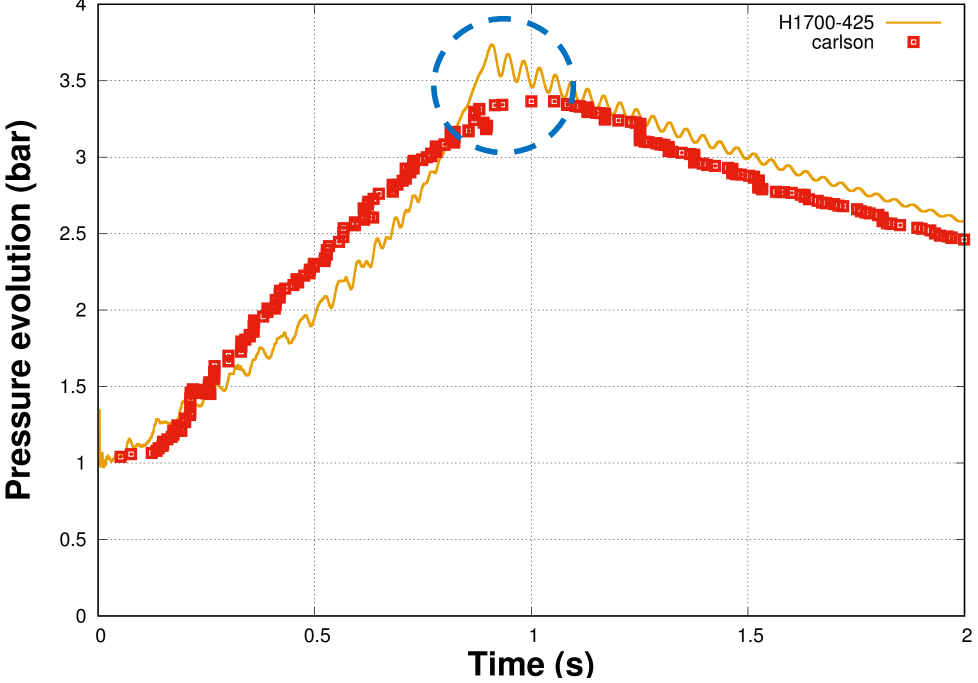
$$\longrightarrow \left(\frac{\boldsymbol{X}}{\boldsymbol{D}}\right)_{\boldsymbol{v=max}} \approx \frac{\mathbf{1}}{\mathbf{2}} \times \frac{\boldsymbol{L}}{\boldsymbol{D}} = \mathbf{15}$$

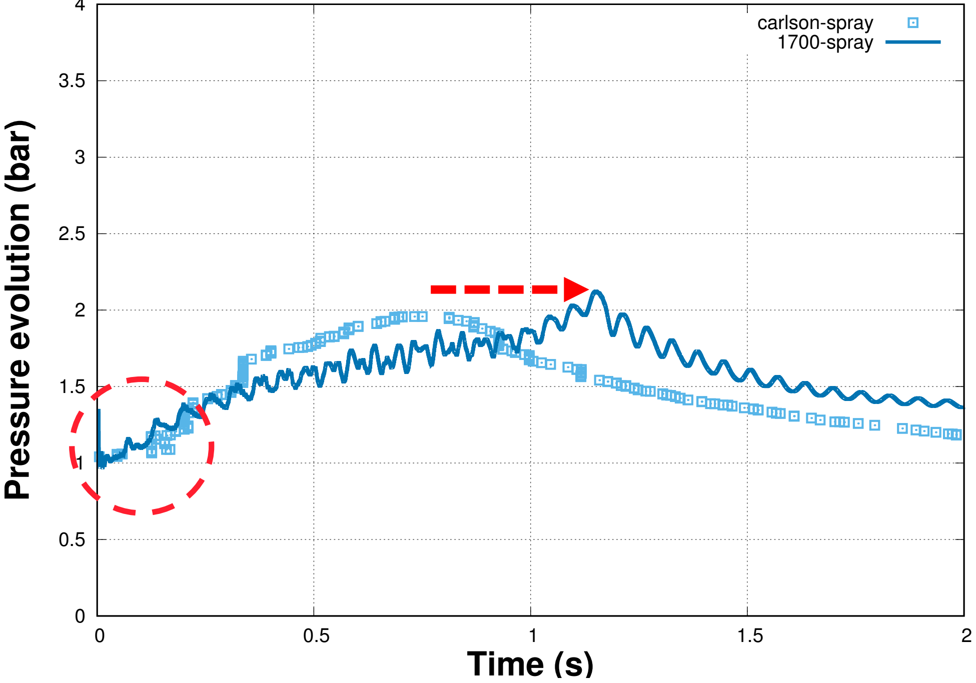
$$\longrightarrow \boldsymbol{v_{max} \leq 70\ m/s}$$

***SLOW** Deflegration Regime*

Maximal Flame Velocity $\boldsymbol{v_{max} \leq 70\ m/s}$

SIMULATION RESULTS


Test 7 No spray


Test 8 With spray

Test	$T_0(K)$	$P_0(atm)$	$T_{liq}(K)$	$\Delta x(m)$	$K_0(m/s)$	$H\ (J/m^3Ks)$	$\dot{\alpha}\ (s^{-1})$
7	298	1.0	-	0.1	5.73	1700	-
8	298	1.0	298	0.1	5.73	1700	6.2×10^{-4}

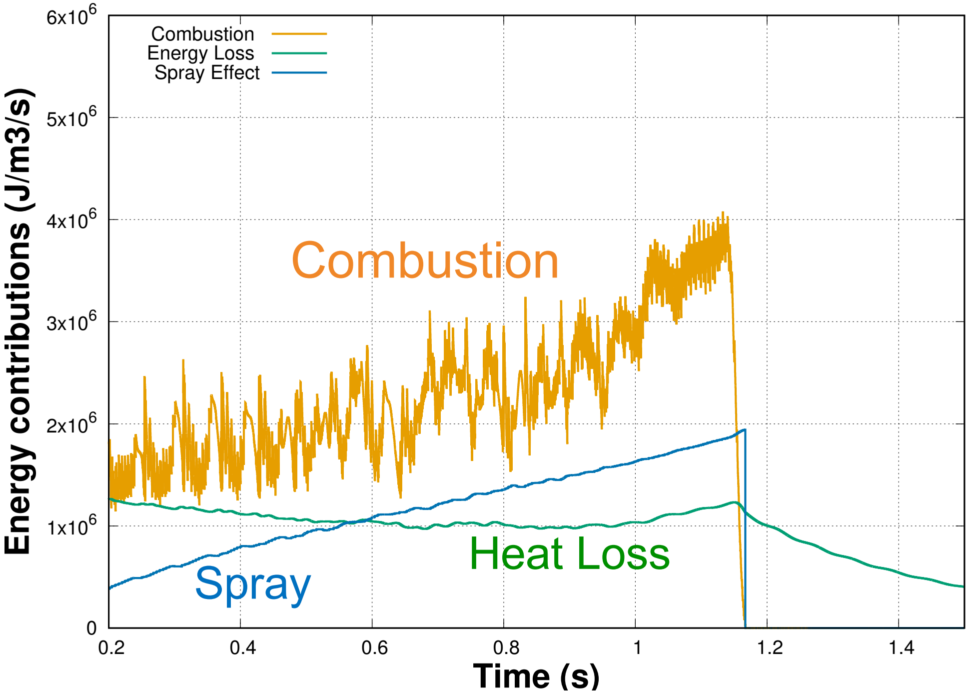
*Experimental geometry with 13 transducers of pressure

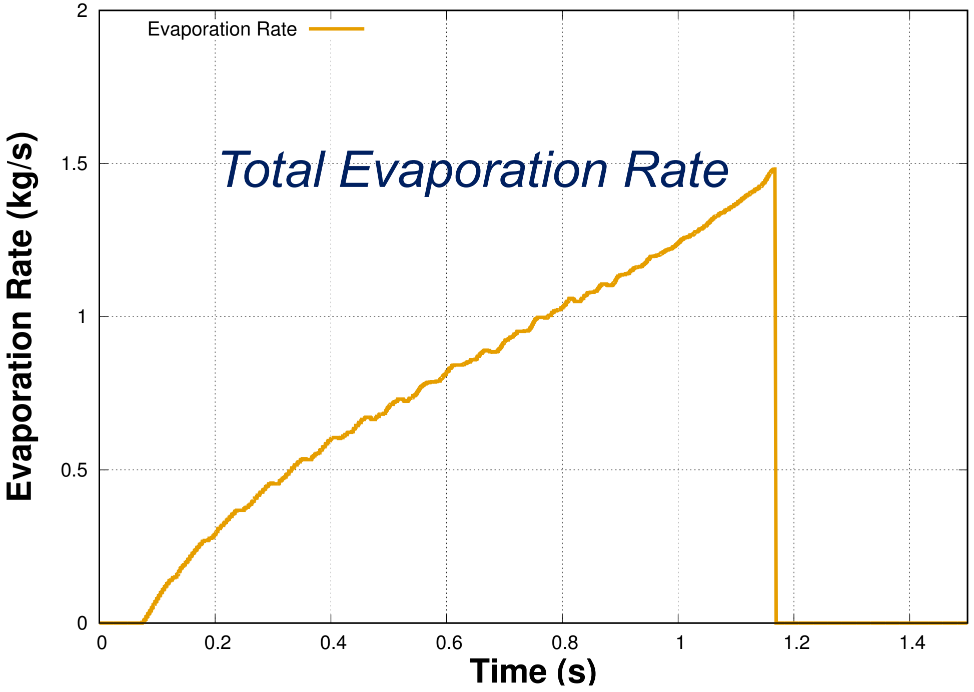
***Suitable* choices for H, K_0 and $\dot{\alpha}$**

***Effective* mitigation effect of spray system**

ENERGY BALANCE

Energy Conservation: $$\frac{d}{dt}\int_V \rho e_t dV = \int_V \boxed{\{\text{combustion}\}} dV + \int_V \boxed{\{\text{convective energy loss}\}} dV + \int_V \boxed{\{\text{evaporation}\}} dV$$





Pressure evolution is associated with energetic evolution

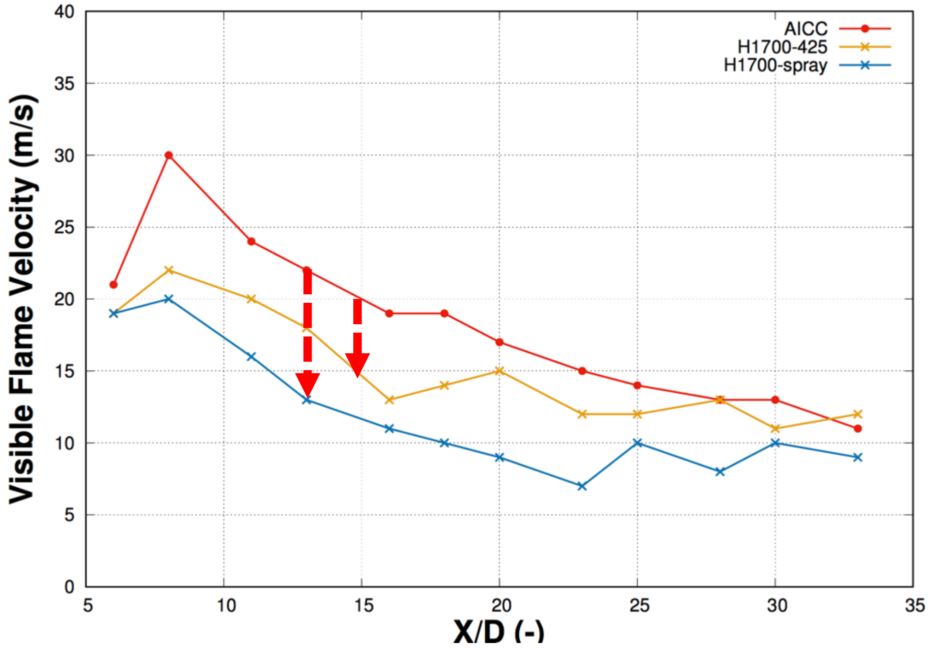
Total **evaporated mass**:

$$m_{H_2O} = N_{evap}\dot{\alpha}\Delta t V_{cell}\rho_{H_2O} \approx 0.825\ kg$$

Mean **evaporation rate**:

$$Q_{evap} = \frac{m_{H_2O}}{t_{tot}} = \mathbf{0.69\ kg/s} < Q_{spray} = 4.6\ kg/s$$

FLAME VELOCITY EVOLUTION

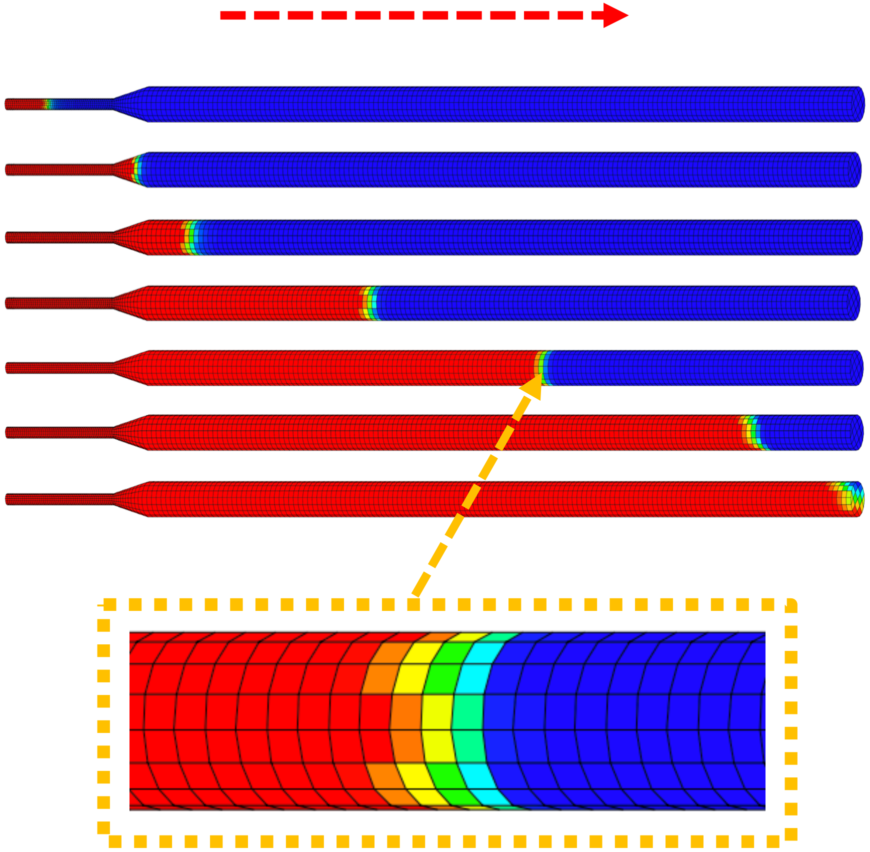


Heat loss : $\Delta v \approx 5\ m/s$

Spray effect : $\Delta v \approx 10\ m/s$

***Effective* deceleration of flame**

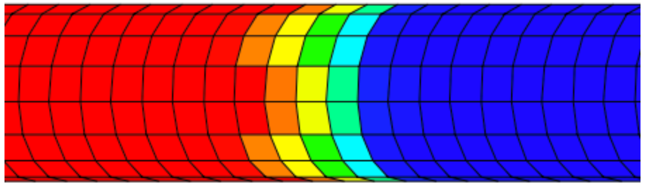
Flame *Propagation Direction*



Flame *Front Sketch*

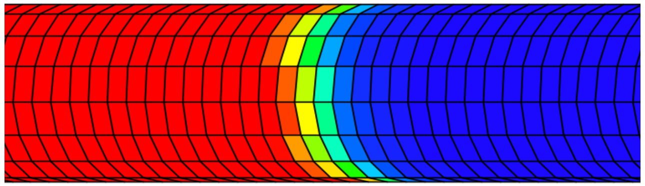
MESH EFFECT

Fig. **Original Mesh**



$\Delta x \approx 10\ cm$

Fig. **Finer Mesh**



$\Delta x \approx 5\ cm$

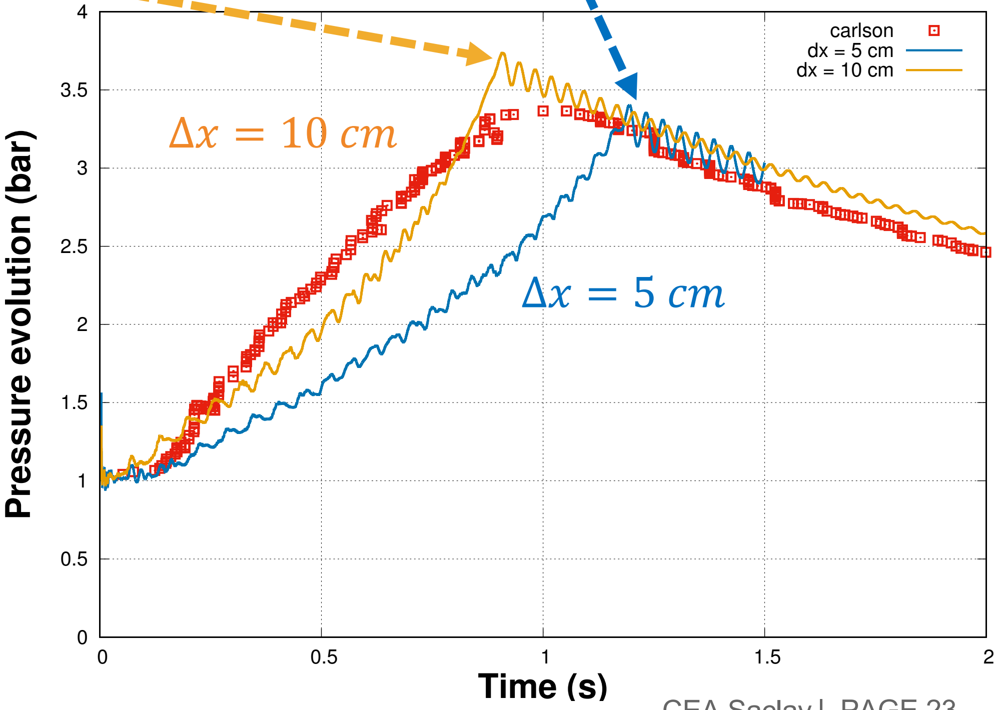
Combustion rate:

$$\dot{\omega}_\xi = \frac{K_0}{\Delta x} \cdot \{\text{criterion function}\}$$

Δx can affect *chemical reaction* rate

K_0 needs to be increased to get the good peak time

Influence on K_0



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Conclusions and Perspectives

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CONSLUSIONS AND PERSPECTIVES

HIGHTLIGHTS:

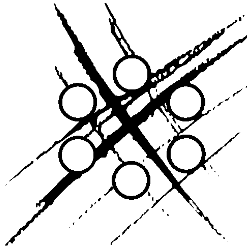
- The lumped-parameter and CFD code can give reliable results for isochore and adiabatic combustion, with or without water spray;
- The depressurization and mitigation effect of spray droplets is demonstrated, with increase of the liquid volume fraction;
- The transient evolution of pressure and flame velocity can be simulated by choosing suitable parameters for the combustion, heat loss and evaporation process.

PERSPECTIVES:

- A more sophisticated model for the parameter K_0 can be proposed, taking into account flame-spray interaction;
- A more sophisticated model for evaporation rate can be proposed, taking into account the diameter of droplets.

OPERATORS IN CAST3M

- DETO
- PRIM KONV PENT
- VARI CALLM CALMU
- MODELISER DOMA DIFF
- PROG CHPO EVOL
- …



More *Miracles* with Cast3M…

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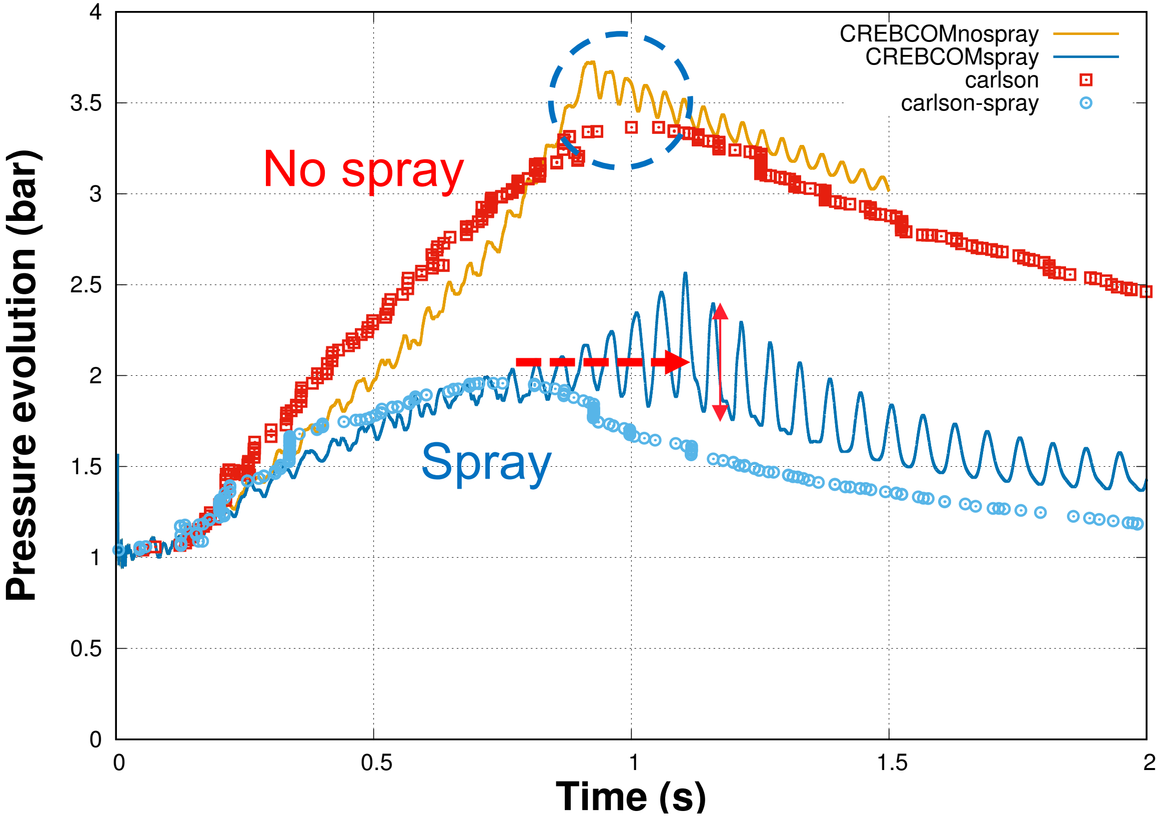
[Malet 2008] J.Malet et al. *Sprays in Containment: Final Results of the SARNET Spray benchmark* Nuclear Engineering & design 25 Sept, **2008**.

MESH EFFECT



***Different** choices for* K_0

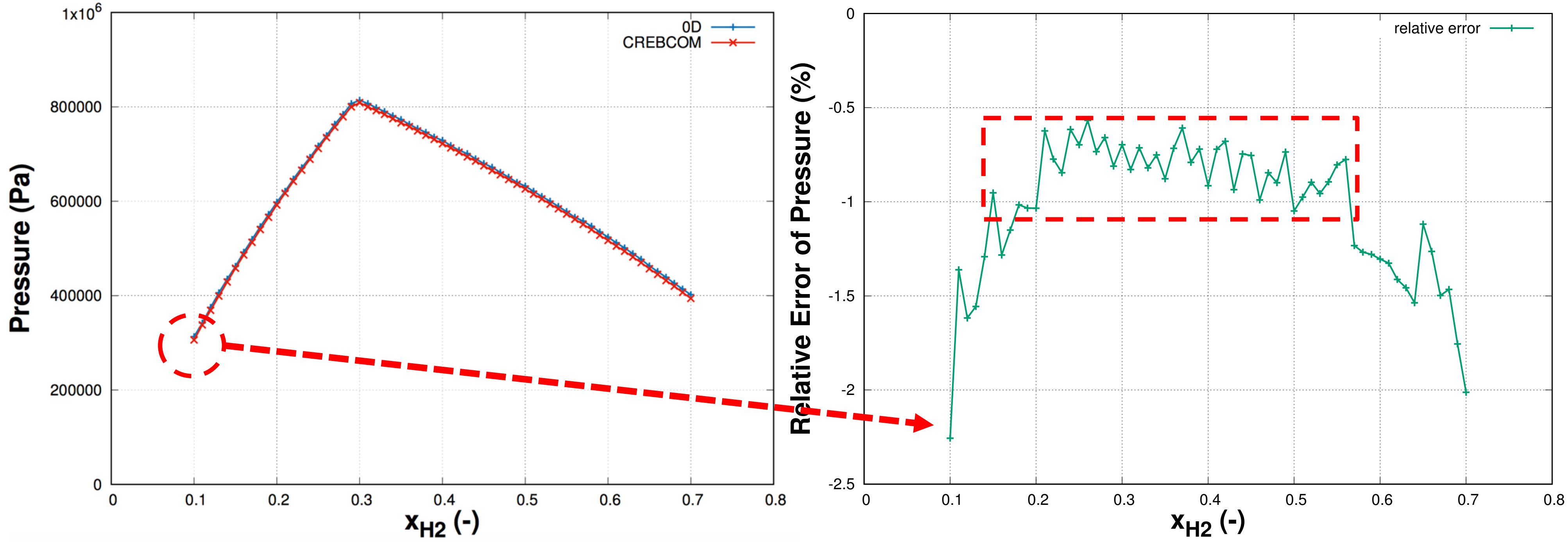
***Effective** mitigation effect of spray system*

*Due to acoustic wave, **oscillation** magnitude increases with* K_0

Test	$T_0(K)$	$P_0(atm)$	$T_{liq}(K)$	$\Delta x(m)$	$K_0(m/s)$	$H\ (J/m^3Ks)$	$\dot{\alpha}\ (s^{-1})$
7	298	1.0	-	0.05	7.0	1700	-
8	298	1.0	298	0.05	7.0	1700	6.2×10^{-4}

*Experimental geometry with 13 transducers of pressure

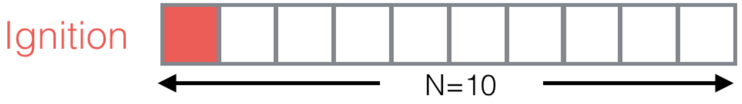
CFD MODEL VALIDATION



Mean values of pressure and temperature are calculated in CREBCOM

Initial conditions	Pressure	Gas temperature	Droplets temperature	Steam concentration	H_2 combustion limit	Volume fraction of droplets
	1.0 atm	293.15 K	293.15 K	0.0	0.4-0.75	2×10^{-4}

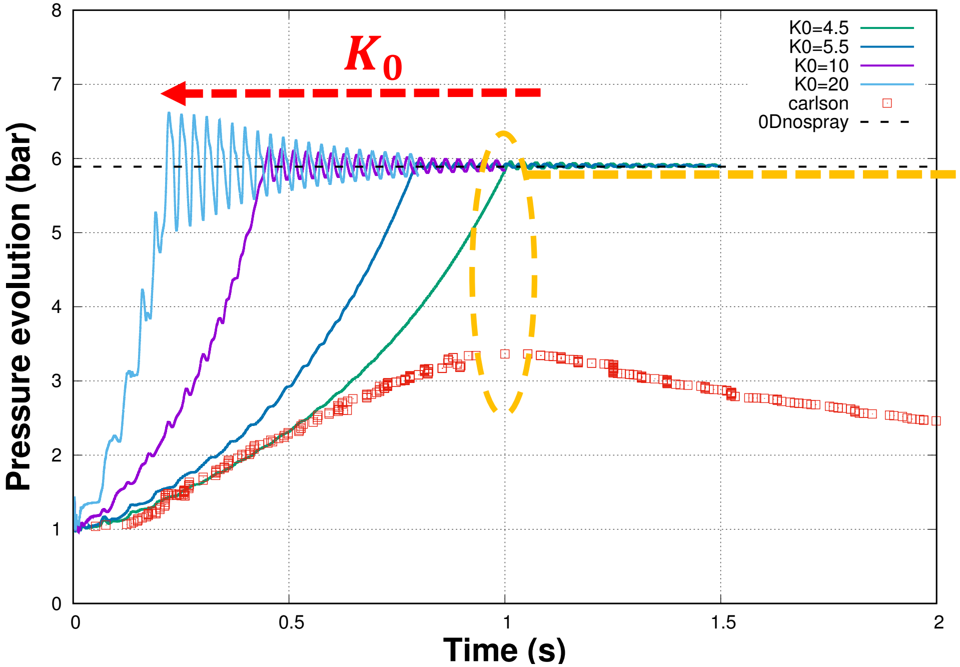
Geometry :



$$\text{Relative error} = \frac{CREBCOM - 0D}{0D} \times 100\%$$

Good coincidence with the lumped-parameter code for the asymptotic ***P*** and ***T***

CHOICE OF K_0 (COMBUSTION RATE)



The *range* of K_0

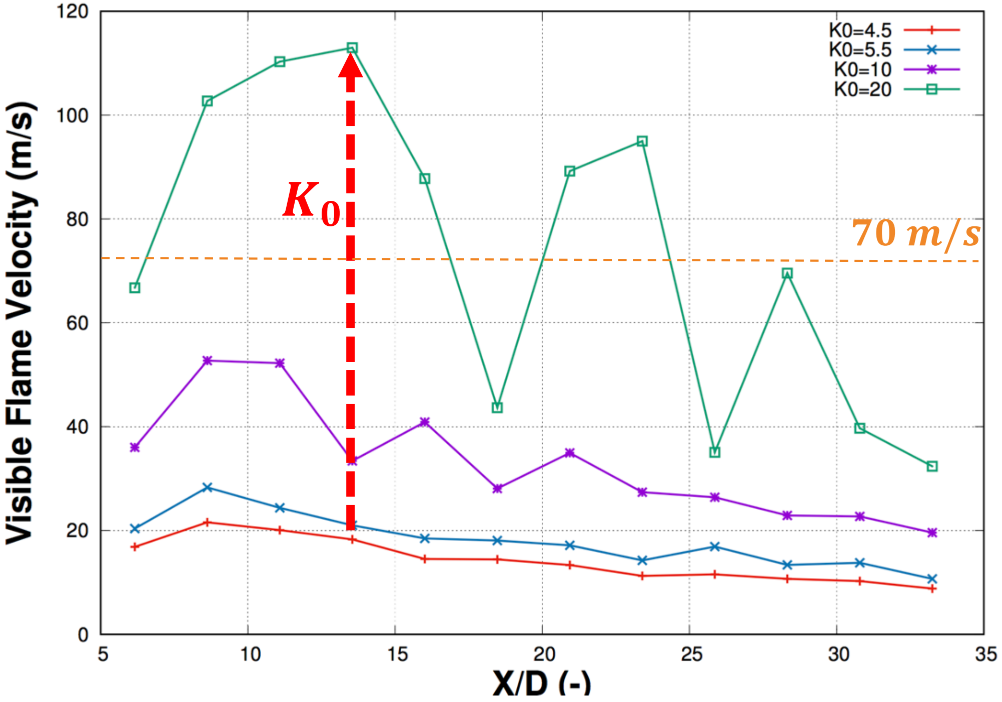
$$4.5\,m/s < K_0 < 10\,m/s$$

$$Flame\ velocity\ v_{flame} \leq 70\,m/s$$

Source: [Efimenko 2001]

$$\frac{S_T}{S_L} = 0.008(\sigma - 1)^3 \left(\frac{L_T}{\delta}\right) \text{ for } \left(\frac{L_T}{\delta}\right) < 500$$

$$K_0 = \frac{S_T(\sigma + 1)}{4} \approx 5.73\mathrm{m/s}$$

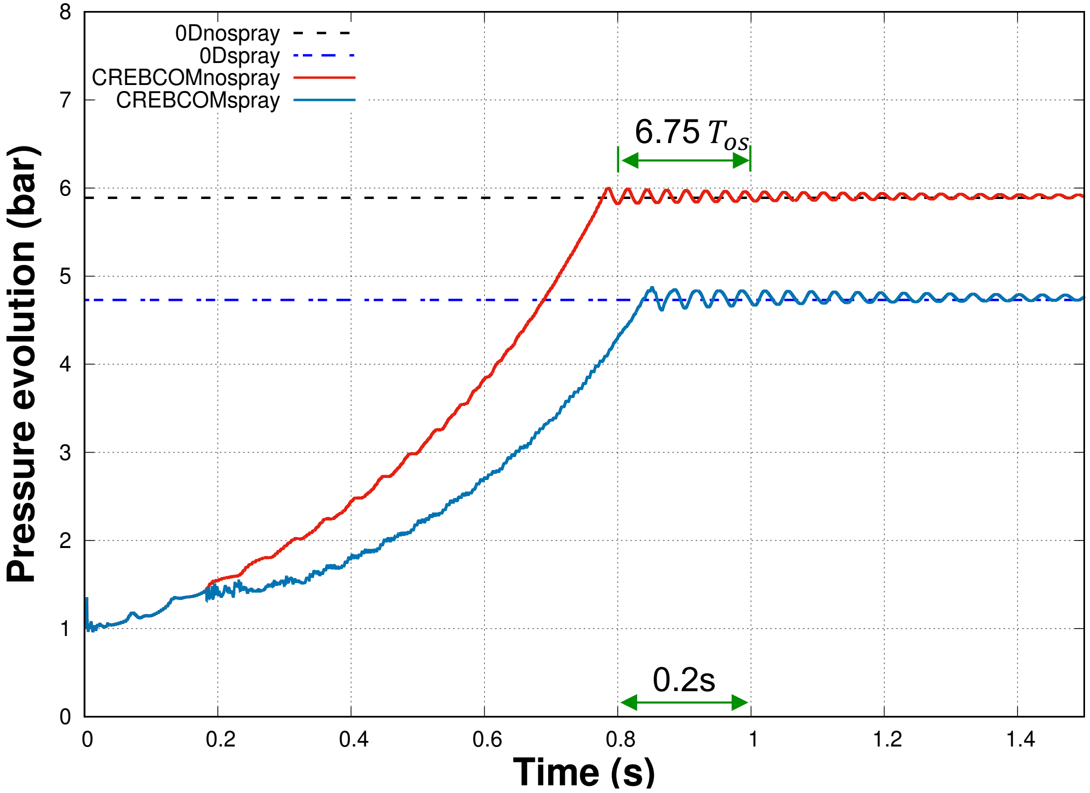


The parameter

$$K_0 = 5.73\,m/s$$

works well *for the* ***available*** *data*

OSCILLATIONS IN PRESSURE EVOLUTION

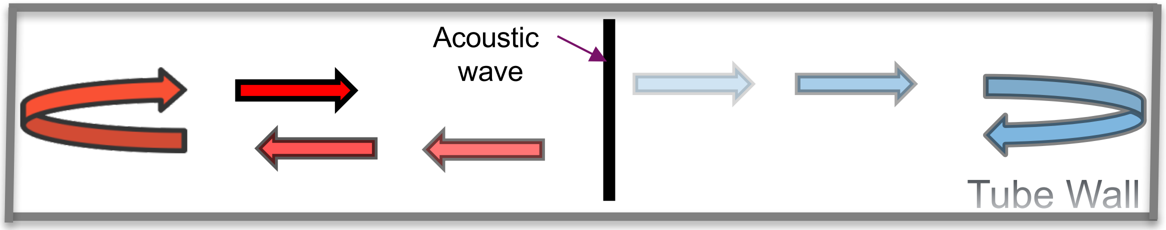


$$6.75\ T_{oscillation} = 0.2\ s$$

$$T_{osscillation} = 2.96\times10^{-2}\ s$$

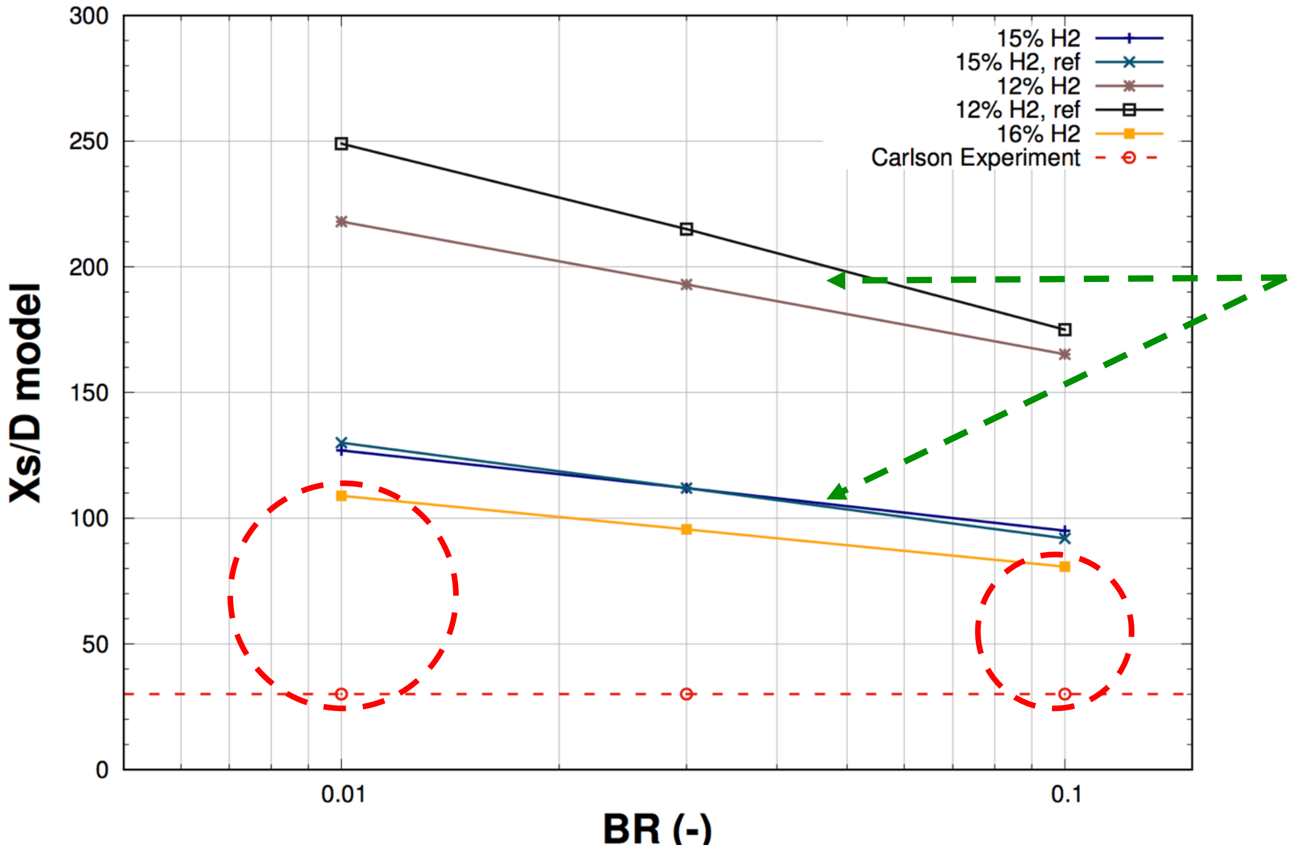
$$T_{acoustic\ wave} = \frac{2\times L}{C_{sp}} \approx 3.1\times10^{-2}\ s$$

$$\boxed{T_{oscillation} = T_{acoustic\ wave}}$$



*The oscillations are due to the **propagation** of the **Acoustic Wave***

RUN-UP DISTANCE



The run-up distance ***Decreases*** with the ***Blockage Ratio***

Validation of correlation

$$\frac{X_S}{D} = \frac{\gamma}{C}\left(\frac{1}{\kappa}\ln\left(\frac{\gamma D}{h}\right)+K\right)$$

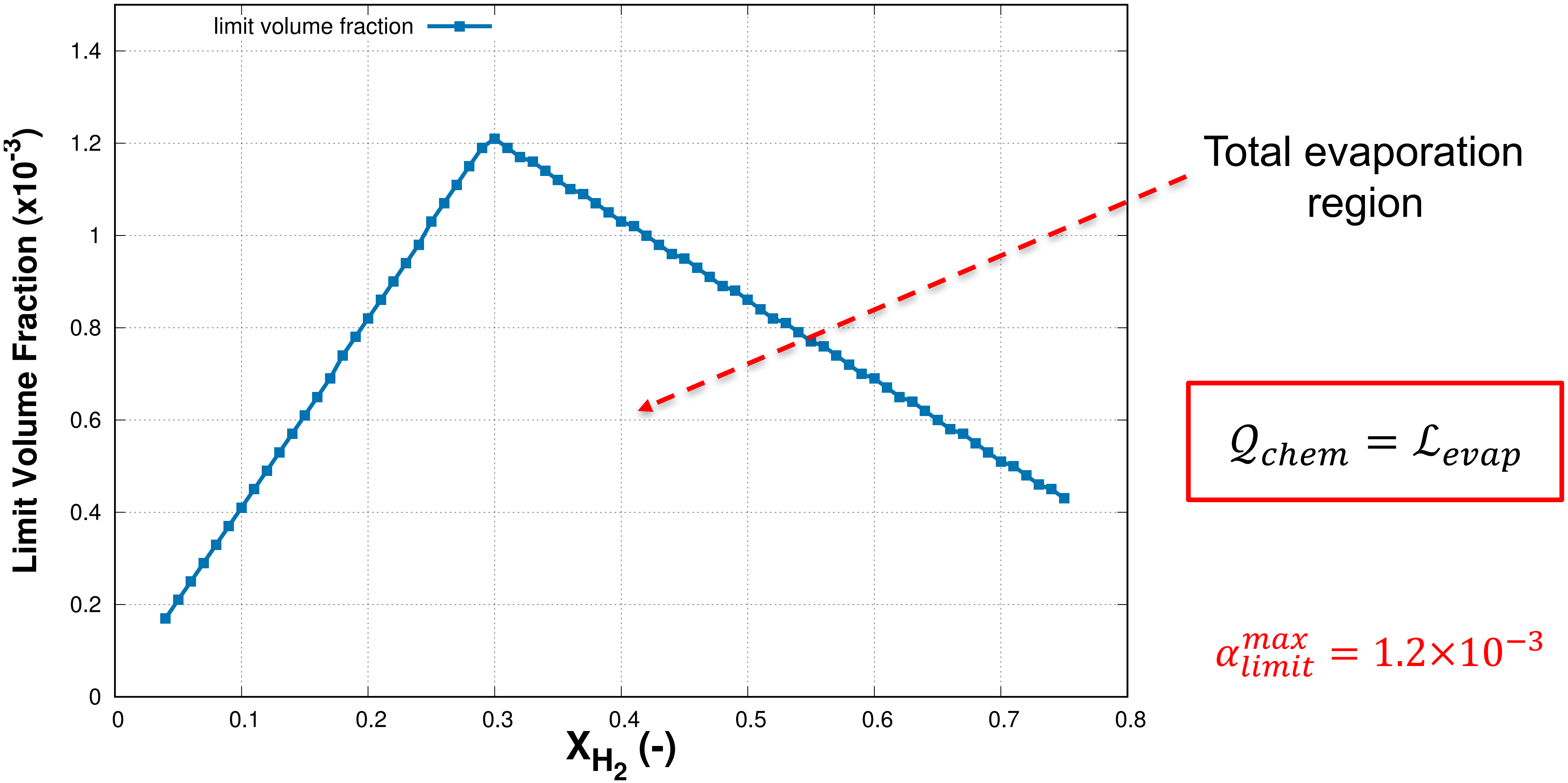
$$\gamma = \left(\frac{c_{sp}}{\mu^2(\sigma-1)^2 S_L}\left(\frac{\delta}{D}\right)^{\frac{1}{3}}\right)^{\frac{3}{6m+7}}$$

$$\frac{D}{h} = \frac{2}{1-\sqrt{1-BR}}$$

Source: [Dorofeev 2009]

Far *from the* ***Run-up Distance***
Smooth tube *in Carlson's experiment*

CASE 2: LIMITING VOLUME FRACTION



Total evaporation region

$$\boxed{\mathcal{Q}_{chem} = \mathcal{L}_{evap}}$$

$$\alpha_{limit}^{max} = 1.2\times10^{-3}$$

$$H_2 + \frac{1}{2}O_2(21\%\ in\ \mathbf{air}) \rightarrow H_2O$$

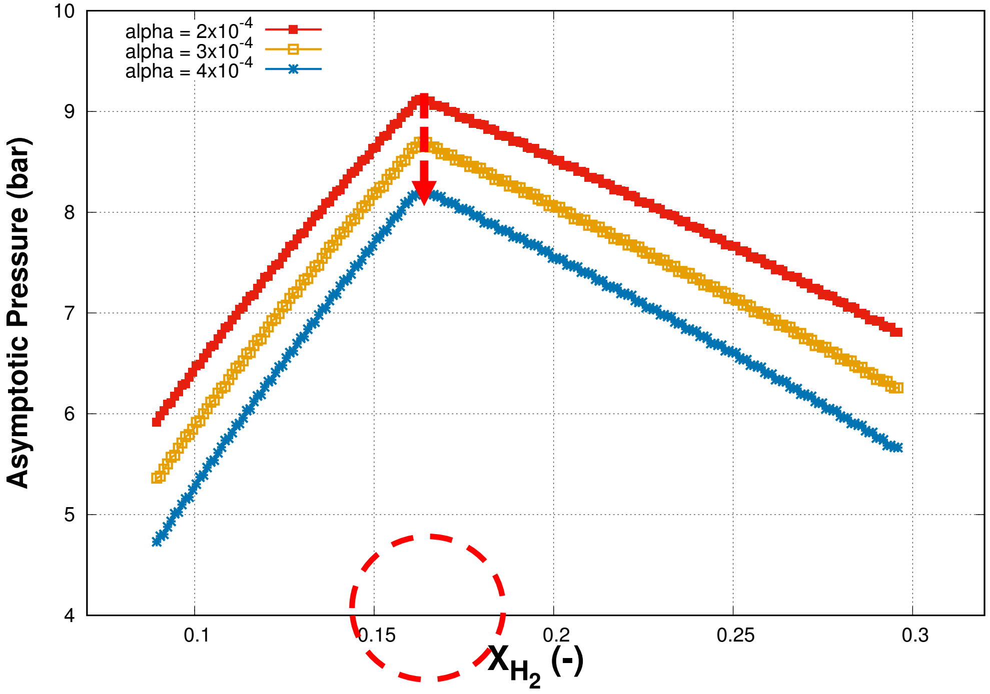
$$H_2O_{liq} \rightarrow H_2O_{vap}$$

CASE 4 : « ACCIDENTAL » CONDITIONS

Source: [Carlson 1973]

Accidental scenario:

Case	$P_{ini}(bar)$	$T_{ini}^{gas}(K)$	$T_{ini}^{liq}(K)$	$X_{H_2}^{ini}(-)$	$X_{H_2O}^{ini}(-)$	$\alpha(-)$
IV	2.4	393.15	293.15	[0.09, 0.3]	0.45	$(2.0, 3.0, 4.0)\times 10^{-4}$



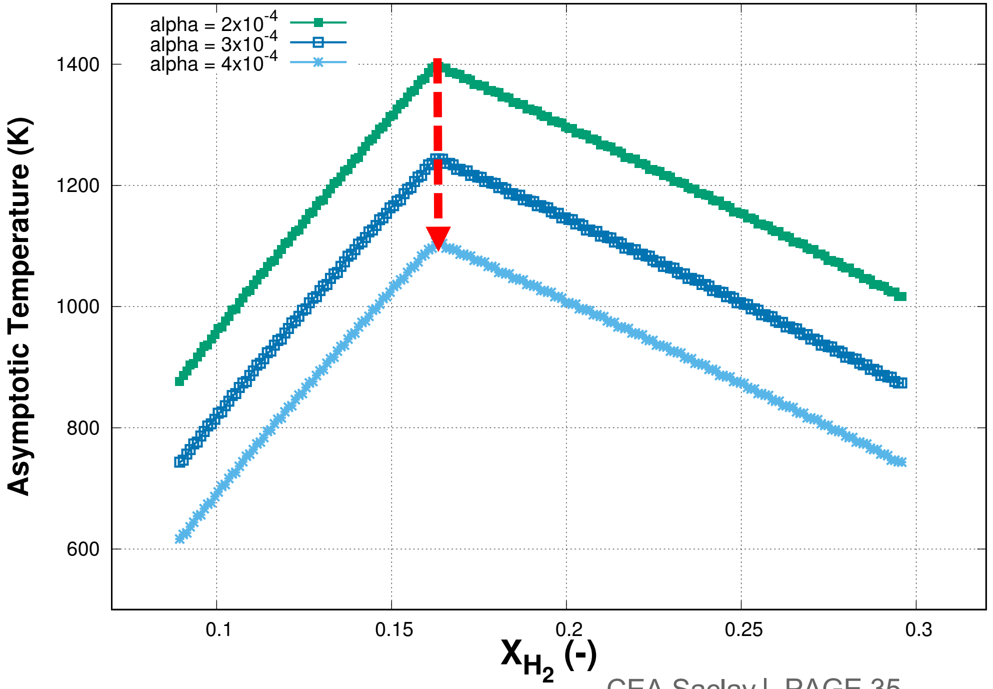
Effective depressurization in accidental scenarios

$$P_{max}^{AICC} = 9.95\ bar$$

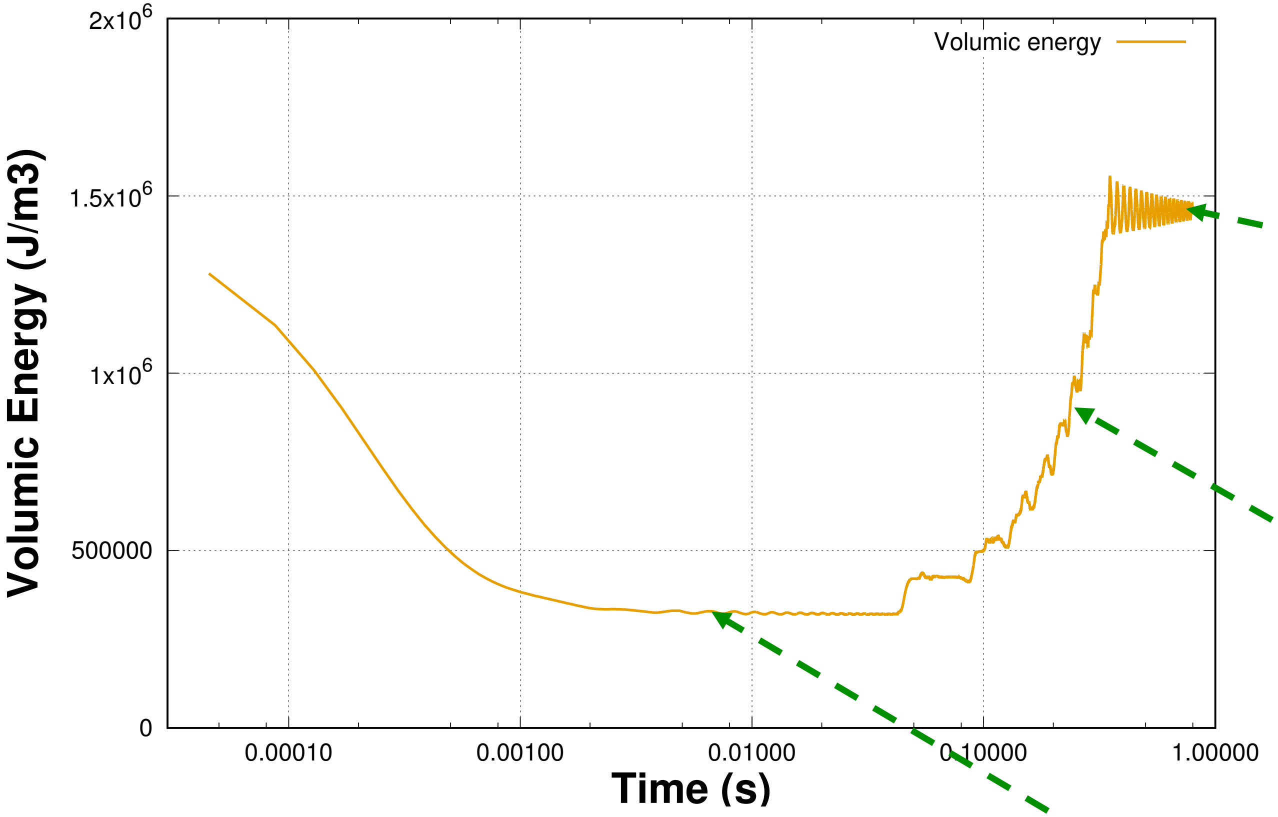
$$P_{max}^{\alpha=4\times10^{-4}} = 8.24\ bar$$

$$T_{max}^{AICC} = 1774\ K$$

$$T_{max}^{\alpha=4\times10^{-4}} = 1104\ K$$



VOLUMETRIC ENERGY EVOLUTION



Close to volumetric energy of **combustion products** in 0D **AICC** calculation

Homogenization Effect due to the **pressure wave** propagation

Thermal Expansion ⇨ **Mass convection**
Leads to the **local decrease** of **volumetric energy**