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PROGRESS IN SAFETY OF HYDROGEN TECHNOLOGIES AND INFRASTRUCTURE:
ENABLING THE TRANSITION TO ZERO CARBON ENERGY

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RAYLEIGH-TAYLOR INSTABILITY: MODELLING AND EFFECT ON COHERENT DEFLAGRATIONS

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Paper ID No: 146

Presentation outline

- Aim and objectives of research.
- Modelling approach.
- H_2-air deflagration at FM Global large scale deflagration chamber.
- Deflagration model results: ‘former’.
- Implementation of Rayleigh-Taylor (RT) instability into model.
- Conclusions.

Introduction

Hydrogen Safety Engineering (HSE):

- Application of scientific and engineering principles to the protection of life, property and environment from adverse effects of incidents/accidents involving hydrogen.

HySAFER Centre at the University of Ulster:

- Understand and predict physical phenomena associated with large scale hydrogen deflagration scenarios.
- Using a Large Eddy Simulation modelling approach.

Aim and objectives

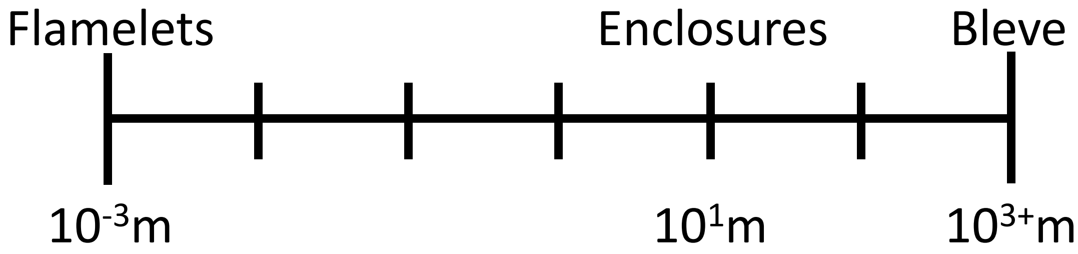
Aim of research:

- Further develop, improve and validate UU Very Large Eddy Simulation (VLES/LES) deflagration model against a broader range of experiments.

Objectives:

- Identify credible combustion enhancing mechanism(s) not accounted for in the current UU VLES/LES deflagration model.
- Implement identified mechanism(s) into model.
- Validate updated model against experiment(s).

LES of deflagrations



- For large scale deflagrations majority of wrinkling is at sub-grid scale (SGS), **“VLES”** approach is implemented.
- For reacting flows the success of this approach requires a **robust turbulent SGS combustion model** (Pope, 2004).
- The successful implementation of the UU multi-phenomena deflagration model depends on both unresolved and partially resolved phenomena.
- UU deflagration model employed using a User Defined Function (UDF) approach, dynamically loaded with ANSYS FLUENT.

UU LES model (1/2)

❖ **Conservation of mass:**

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}.\tilde{u}_j\right) = 0$$

❖ **Conservation of momentum:**

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{u}_i\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right) + \bar{\rho} g_i$$

❖ **Conservation of energy:**

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}\left(u_j \rho E\right) + \frac{\partial p}{\partial x_j} =$$

$$\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}.C_p}{\mathrm{Pr}_{eff}}\frac{\partial T}{\partial x_j} - \sum h_m\left(-\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial Y_m}{\partial x_j}\right) + \mu_{eff}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_i}{\partial x_i}\delta_{ij}\right)\right) + S_e$$

UU LES model (2/2)

- Premixed flame front propagation, progress variable:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{c}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial\tilde{c}}{\partial x_j}\right)+\overline{S}_c$$

- Using gradient method for source term: $\overline{S_c}=\rho_u S_t \left\|\overrightarrow{grad}(\tilde{c})\right\|$

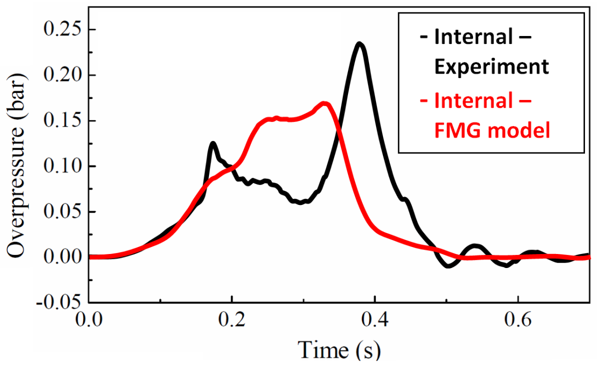
- 'Former' UU deflagration model is based on the interaction of four mechanisms responsible for the increase of flame front surface area. Model is implemented using a ***modified*** version of Yakhot's equation for turbulent flame propagation velocity.
  - **Flow turbulence**
  - **Turbulence generated by the flame front itself, Ξ_k**
  - **Leading points (curvature radius & preferential diffusion), Ξ_{lp}**
  - **Fractal-like flame wrinkling, Ξ_f**

$$S_t = S_u \cdot \exp\left(u'/S_t\right)^2 \Longrightarrow S_t = [S_u \cdot \Xi_K \cdot \Xi_{lp} \cdot \Xi_f]\cdot \exp(u'/S_t)^2$$

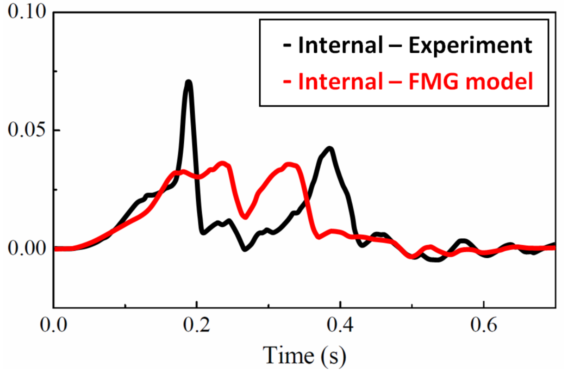
Previous validations

- Model has been successfully validated against:
  - **Large-scale hydrogen-air deflagrations in closed vessels with uniform and non-uniform mixtures.**
  - **Largest known unconfined experiments.**
  - **78.5m long tunnel.**
- Application of the 'former' version of UU deflagration model, when compared to FMG vented deflagration experiments, led to under-prediction of overpressures.
- FM Global modelling approach also did not ***initially*** replicate experimental overpressures.

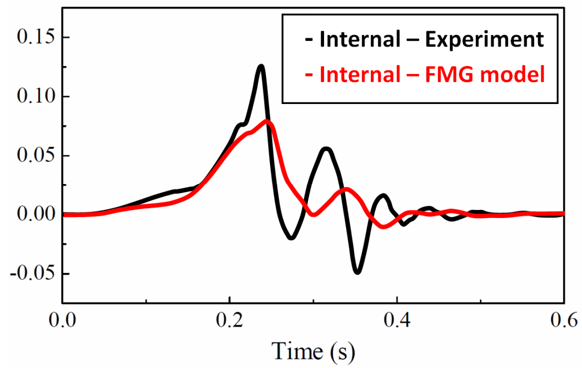
Central ign. / 2.7m^2 vent



Central ign. / 5.4m^2 vent



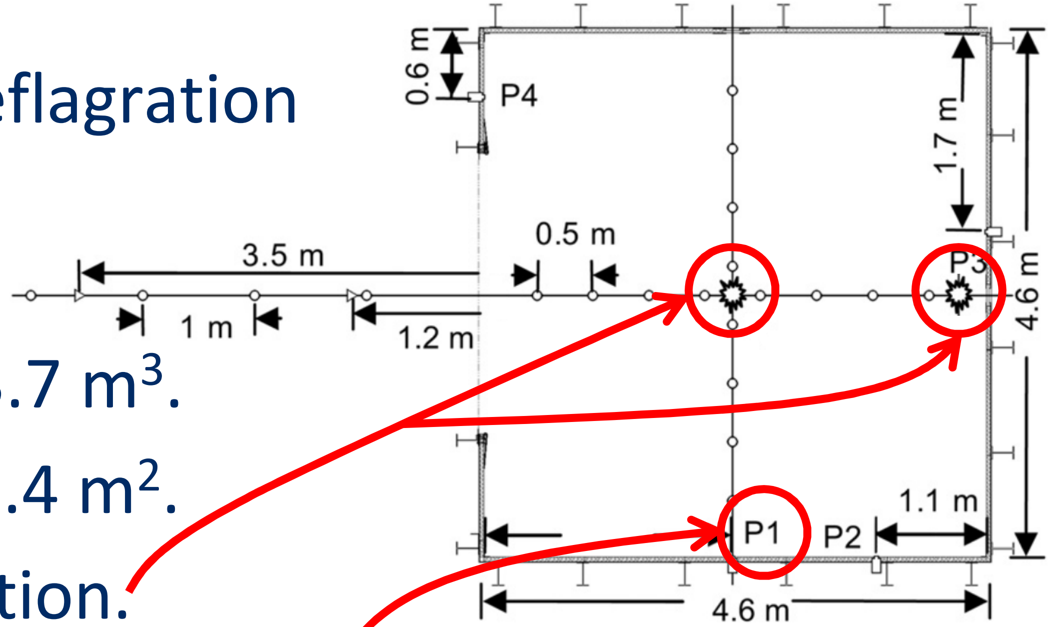
Back wall ign. / 5.4m^2 vent



Bauwens et al., 3rd International Conference on Hydrogen Safety, Corsica, 2009

FM Global experiment

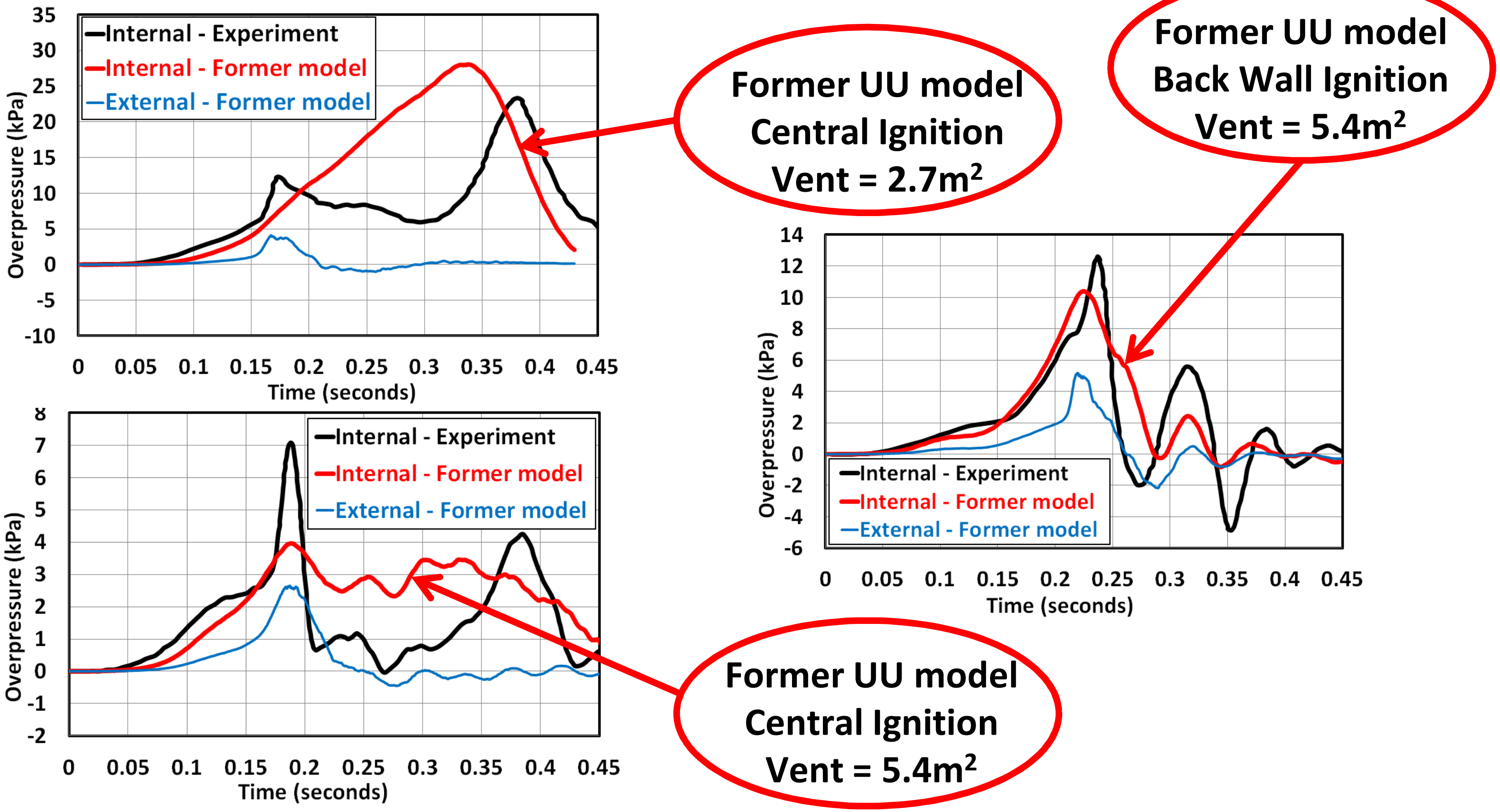
- FM Global large scale deflagration chamber.
- Chamber dimensions: 4.6 m x 4.6 m x 3 m = 63.7 m^3.
- Square vent: 2.7 m^2 or 5.4 m^2.
- Central or back wall ignition.
- 18 % vol. hydrogen-air mixture.
- 4 internal pressure transducers.
- Pressure data obtained from loc. P1.



Bauwens et al., International Journal of Hydrogen Energy, 36, pp. 2329-2336, 2011

Former model results

Results from unmodified deflagration model:



Rayleigh-Taylor instability

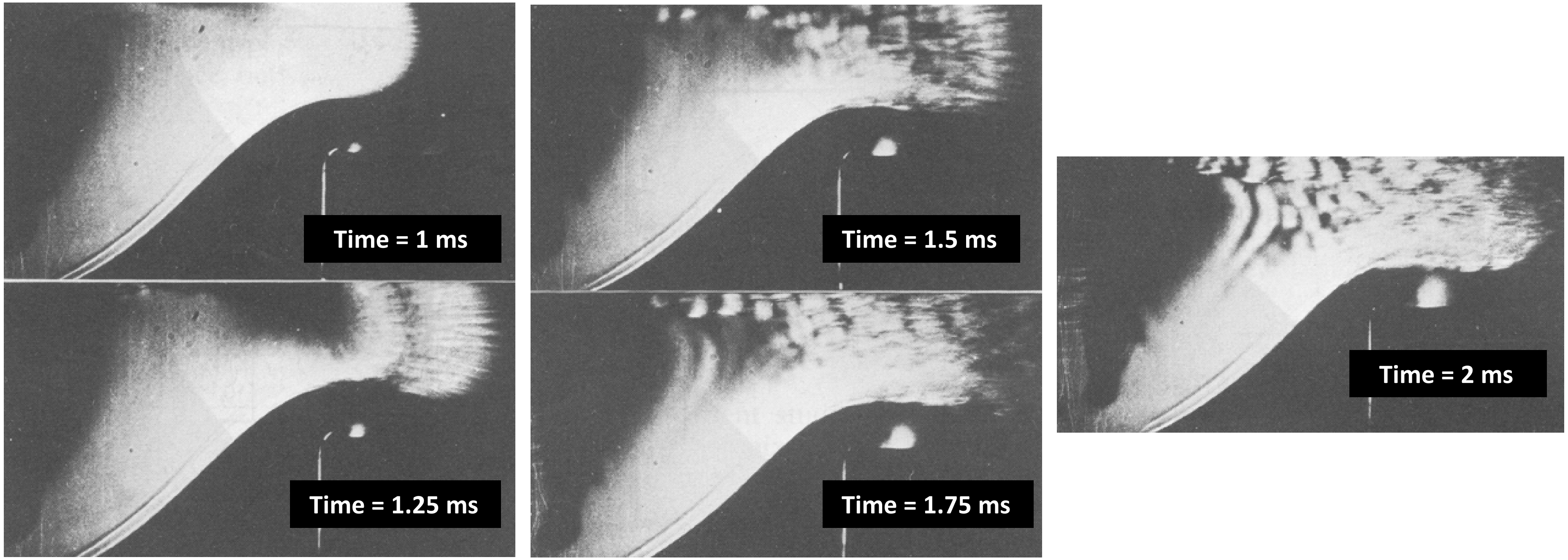
- Rayleigh-Taylor (RT) instability identified as missing mechanism, which would if implemented into UU LES deflagration model increase flame front area.
- RT instability occurs at the interface between two fluids, subject to acceleration in the direction from the lighter to the heavier.
- In a propagating flame:
    - Unburned mixture – heavier fluid.
    - Combustion products – lighter fluid.
- ***"Depending on the layout of the vent arrangement and the point of ignition, RT instability may dominate all other mechanisms that commonly are believed to be important in governing pressure build-up"***

Solberg et al., Eighteenth Symposium (International) on Combustion, pp. 1607-1614, 1981

Experimental observation

Growth of flame front turbulence investigated by Tsuruda & Hirano:

Tsuruda and Hirano, Combustion Science and Technology, 51 (4-6), pp. 323-328, 1987



- Obstacle placed in path of flame inside combustion chamber.
- Acceleration induced just before flame front passed obstacle.
- Flame front became ***needle-like*** in structure.
- For this experimental setup acceleration induced mechanism - dominant over all mechanisms which increase flame surface area.

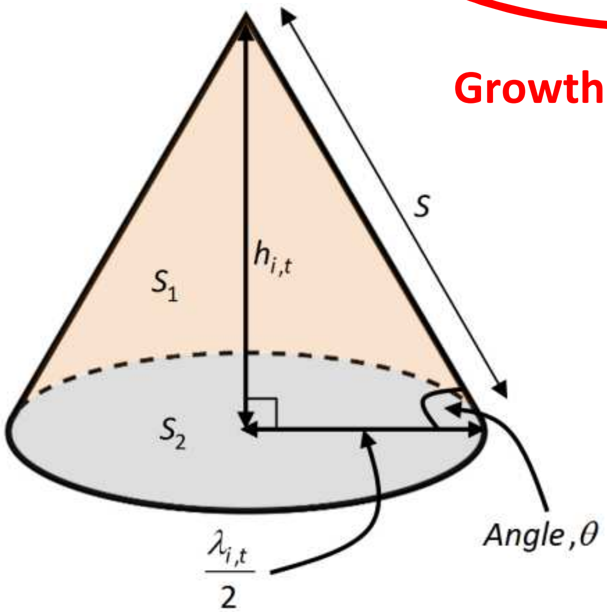
RT model (1/3)

Calculation of RT perturbation amplitude, $h_{i,t}$:

$$h_{i,t} = h_{i,t-\Delta t}\left(1+\omega_{i,t}\cdot\Delta t\right) - \alpha\cdot S_{t,i,t}\left(\Xi_{RT}-1\right)\Delta t$$

Growth of perturbation

Removal of RT flame wrinkling – 'Sink'



- **Wavelength:** $\lambda_{i,t} = 4\cdot\pi\cdot\left(\frac{v_{T,i,t}^2}{Acc_{i,t}\cdot Atw_{i,t}}\right)^{1/3}$

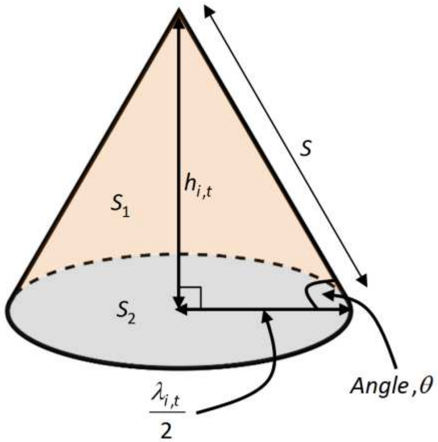
  Youngs, D. L., Physica 12D, Netherlands, 1985, pp. 32-44

- **Atwood number:** $Atw_{i,t} = \frac{\left(\rho_{u,i,t}-\rho_{b,i,t}\right)}{\left(\rho_{u,i,t}+\rho_{b,i,t}\right)}, \rho_{u,i,t} > \rho_{b,i,t}$

- **Growth rate:** $\omega_{i,t} = \sqrt{Atw_{i,t}\cdot\frac{2\pi}{\lambda_{i,t}}\cdot Acc_{i,t}}$

- **Acceleration:** Calculated within each control volume, per timestep, in the direction normal to the propagating flame front.

RT model (2/3)



$$\Xi_{RT} = \frac{S_1}{S_2} = \frac{\pi \cdot \left(\frac{\lambda_{i,t}}{2}\right) \cdot \sqrt{\left(\frac{\lambda_{i,t}}{2}\right)^2 + h_{i,t}^2}}{\pi \cdot \left(\frac{\lambda_{i,t}}{2}\right)^2} = \frac{\sqrt{\left(\frac{\lambda_{i,t}}{2}\right)^2 + h_{i,t}^2}}{\left(\frac{\lambda_{i,t}}{2}\right)}$$

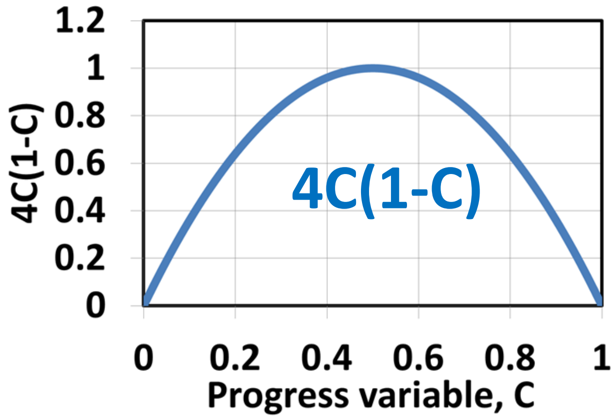
Source term, $\frac{d\,\Xi_{RT}}{dt}$, generation and suppression of RT instability:

- $$\frac{d\,\Xi_{RT}}{dt} = \frac{d\,\Xi_{RT}}{dh} \times \frac{dh}{dt}$$ $$h_{i,t} = f\left(\sqrt{(\Xi_{RT} - 1)}\right)$$
- $$\frac{d\,\Xi_{RT}}{dh} = RT \frac{2 \cdot h_{i,t}}{\lambda_{i,t}\sqrt{\left(\frac{\lambda_{i,t}}{2}\right)^2 + h_{i,t}^2}}, \quad \frac{dh}{dt} = \left(h_{i,t} \cdot \omega_{i,t}\right) - \alpha \cdot S_{t,i,t}\left(\Xi_{RT} - 1\right)$$

RT model (3/3)

- **Unsteady term:** Accumulation of Ξ_{RT} in each CV.
- **Convection term:** Transport of Ξ_{RT} due to velocity field.
- **Source term:** Accounts for sources and sinks, which either create or destroy Ξ_{RT} :
  - $S_{\Xi RT} = (Growth_{RT} - Sink_{RT})$ x $[4C(1\text{-}C)]$
  - Multiplier added to limit Ξ_{RT} growth outside the flame.

$$\underbrace{\frac{\partial \Xi_{RT}}{\partial t}}_{\text{Unsteady term}} + \underbrace{\left(U_i + S_{t,i}\right)\cdot \frac{\partial \Xi_{RT}}{\partial x_i}}_{\text{Convection term}} = \underbrace{S_{\Xi_{RT}}}_{\text{Source term}}$$



Weller et al., Flow, Turbulence and Combustion, 72, pp. 1-28, 2004

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Model parameters

RT model contains two user-defined parameters: k_h & α

1. Initial amplitude of flame instability – k_h:

- To calculate initial RT amplitude inside CV 'i': $h_{0,i,t} = k_h \times \lambda_i$
- Influence of RT limited to the area of the external deflagration:
  - In the key area of interest, $k_h = 0.5$.
  - In all other locations, $k_h = 0.001$.

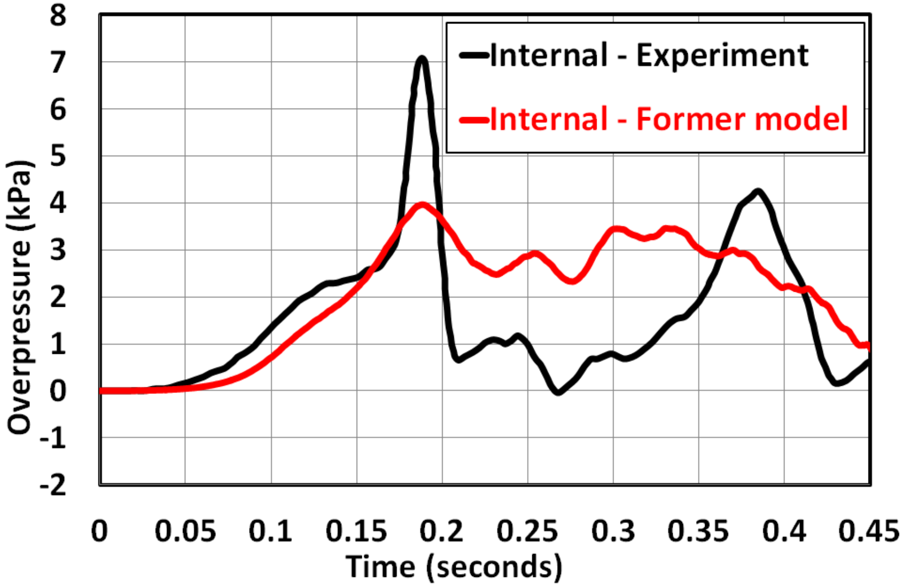
2. Surface 'Sink' term – α:

- Constant multiplier to increase or decrease removal rate.
- If term set to 1.0 – α has no influence on consumption rate.
- Following parametric analysis α set to 0.75.

$$h_{i,t} = \underbrace{h_{i,t-\Delta t}\left(1+\omega_{i,t}\cdot\Delta t\right)}_{\text{Growth of perturbation}} - \underbrace{\alpha\cdot S_{t,i,t}\left(\Xi_{RT}-1\right)\Delta t}_{\text{Removal of RT flame wrinkling – 'Sink'}}$$

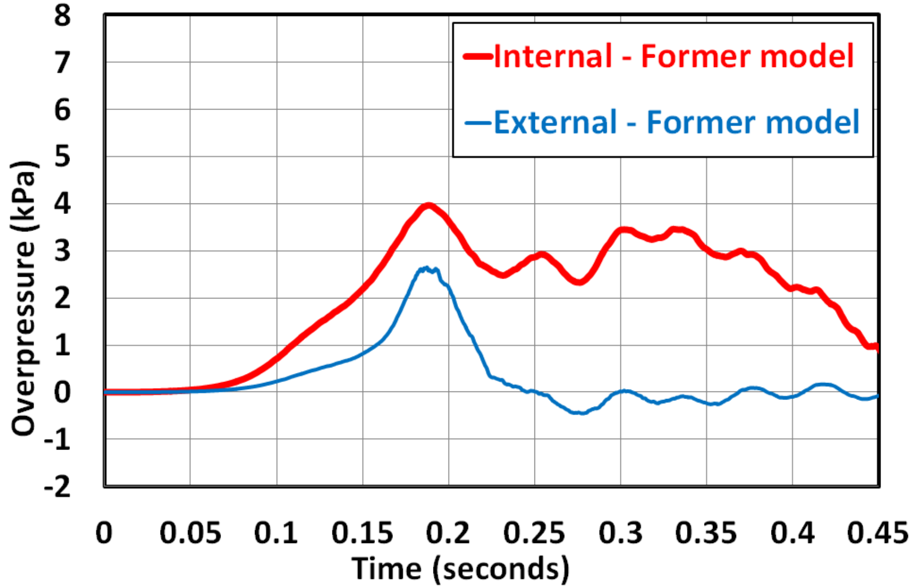
Former model result, central ignition, 5.4 m² vent

Internal



- ‘Former’ model failed to reproduce first distinct pressure peak.
- This internal pressure peak is caused by external deflagration.

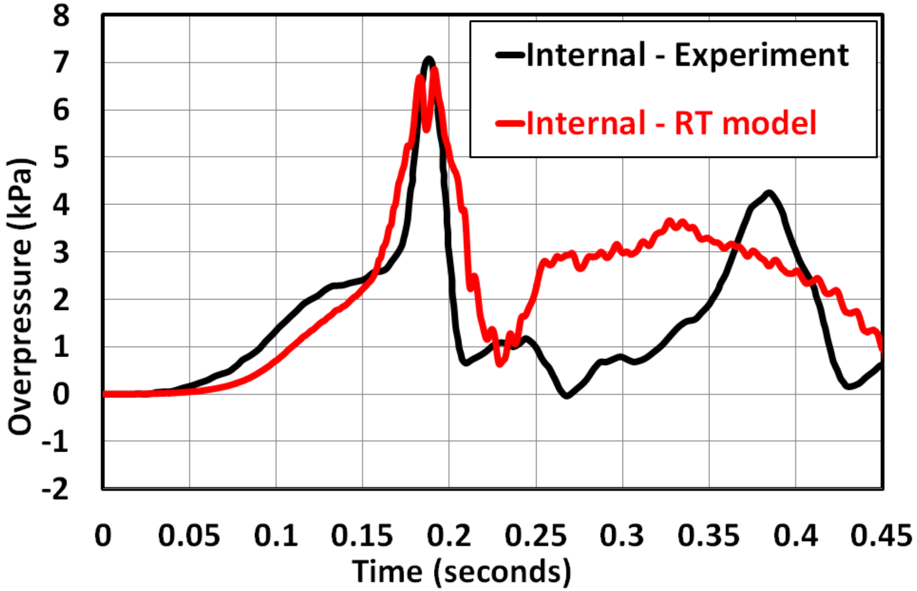
External



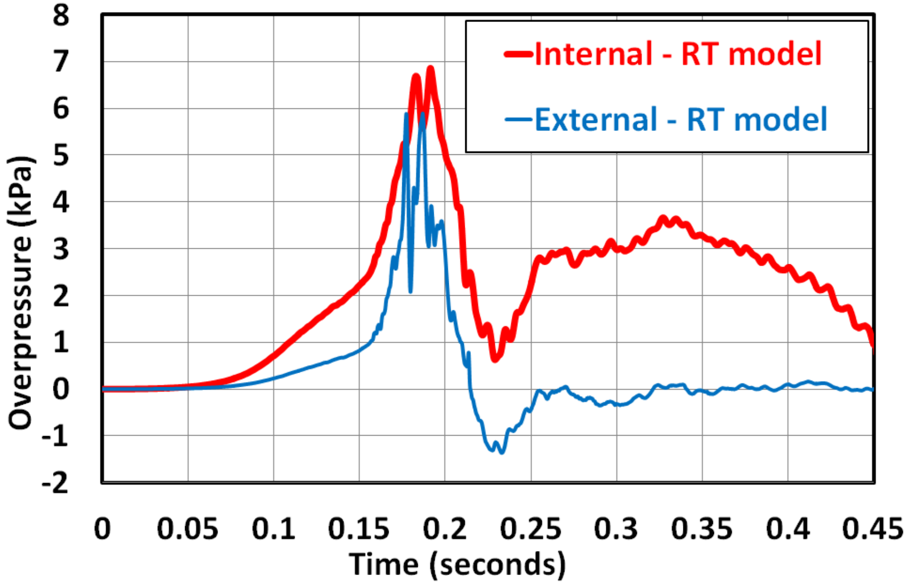
- External pressure less than internal pressure.
- To have influence, external pressure should be at least comparable to internal pressure

RT model result, central ignition, 5.4 m² vent

Internal



External

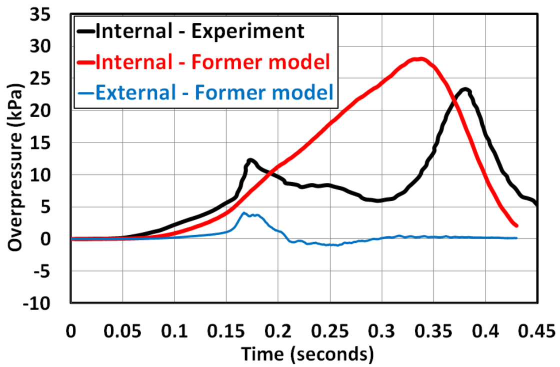


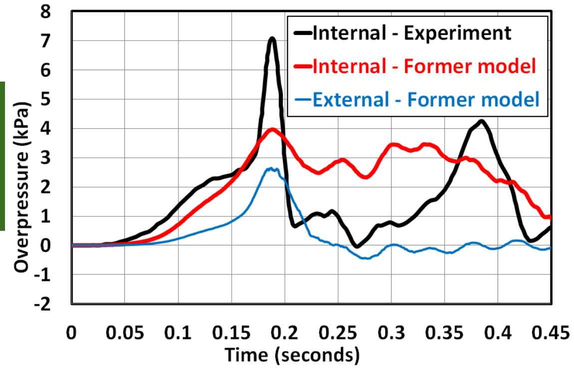
- Intensification of external deflagration,
- Associated internal pressure peak reproduced.
- Partial vacuum following dissipation of external deflagration,
- Reduction of internal pressure following first pressure peak.

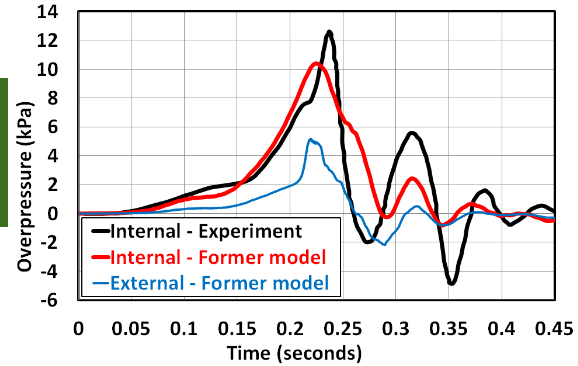
'Former' model vs. RT model

Central ign. / 2.7m² vent	Central ign. / 5.4m² vent	Back wall ign. / 5.4m² vent

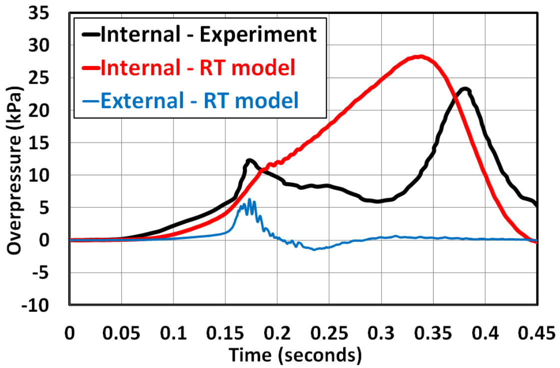
Former model results:

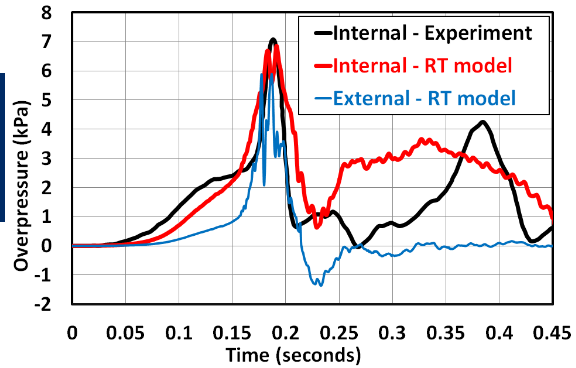


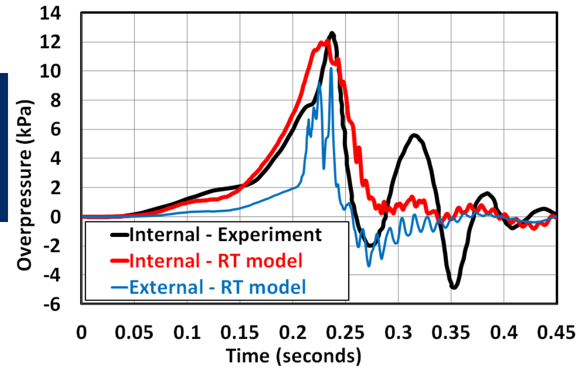




RT model results (in area of external deflagration, $k_h = 0.5$):

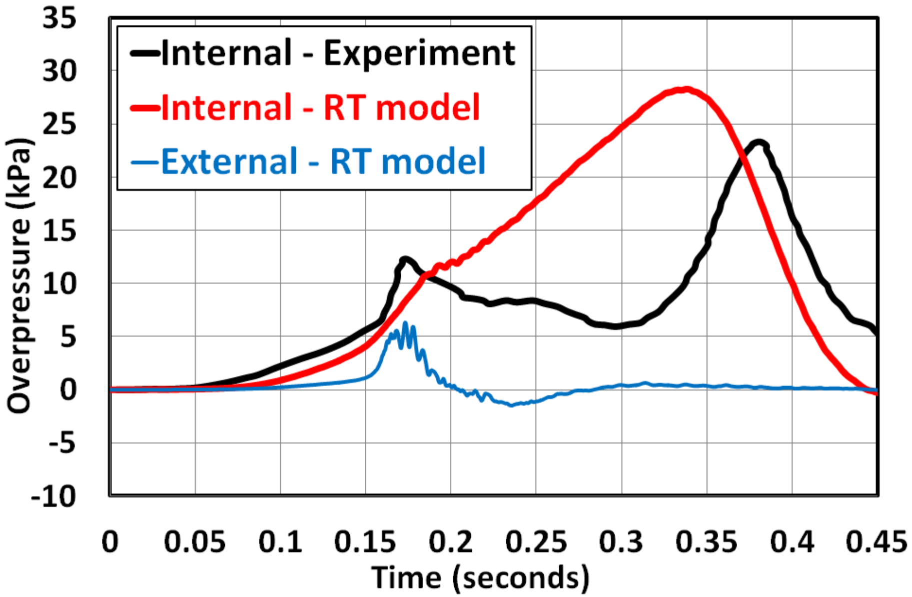






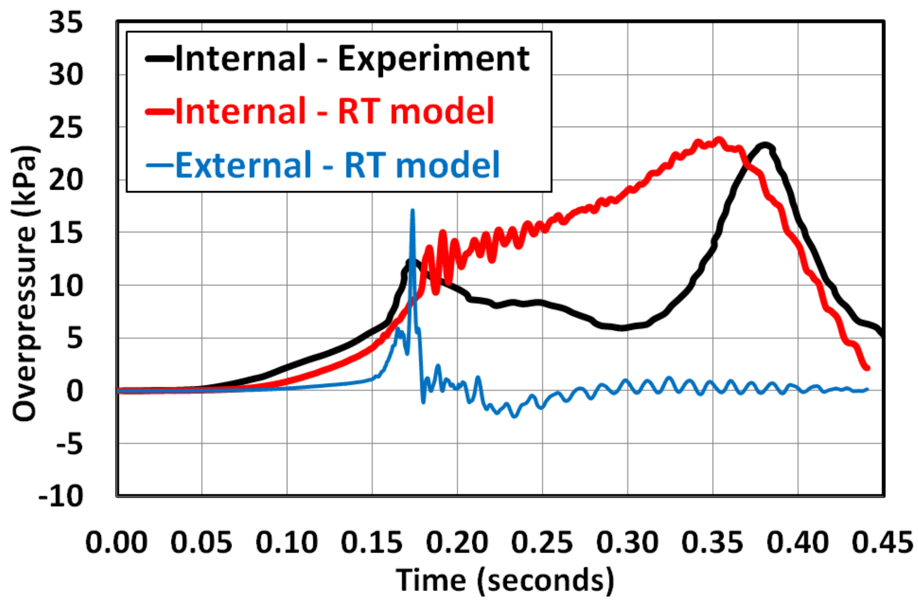
RT model result, central ignition, 2.7 m² vent

RT model result, in area of external deflagration, k_h = 0.5:



Inside Chamber		Outside Chamber	
k_h	α	k_h	α
0.001	0.75	0.5	0.75

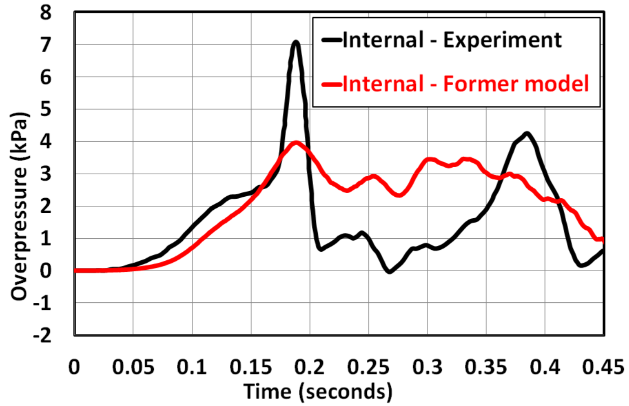
RT model result, in area of external deflagration, k_h = 0.75:



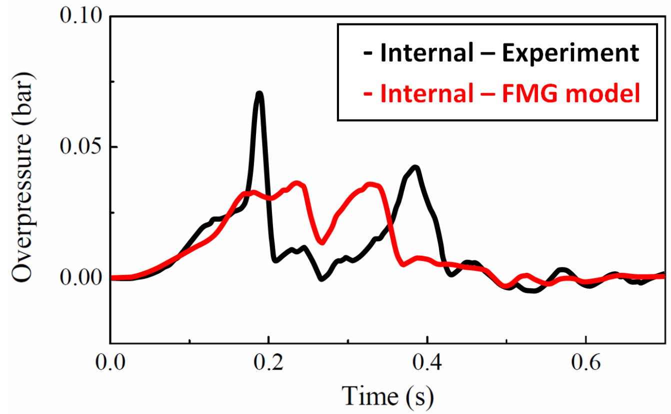
Inside Chamber		Outside Chamber	
k_h	α	k_h	α
0.001	0.75	0.75	0.75

Comparison of result

Former UU model result

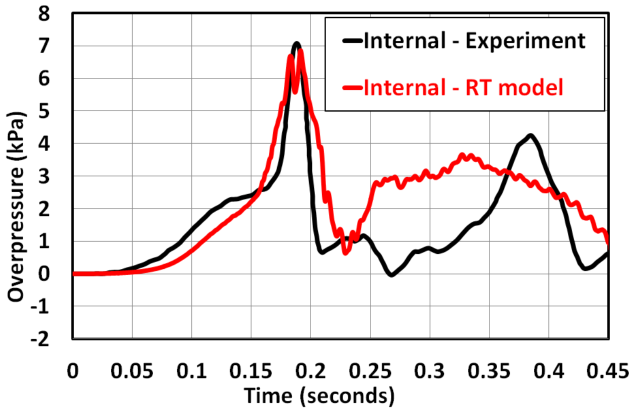


Former FMG model result

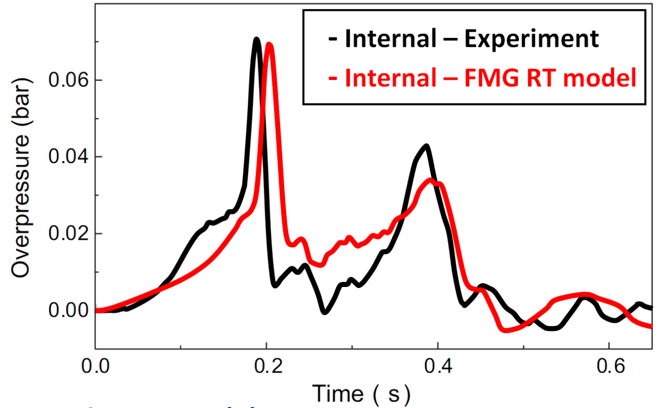


Bauwens et al., 3rd ICHS, Corsica, 2009

UU RT model result



FMG RT model result



Bauwens et al., IJHE, 36(3), pp. 2329-2336, 2011

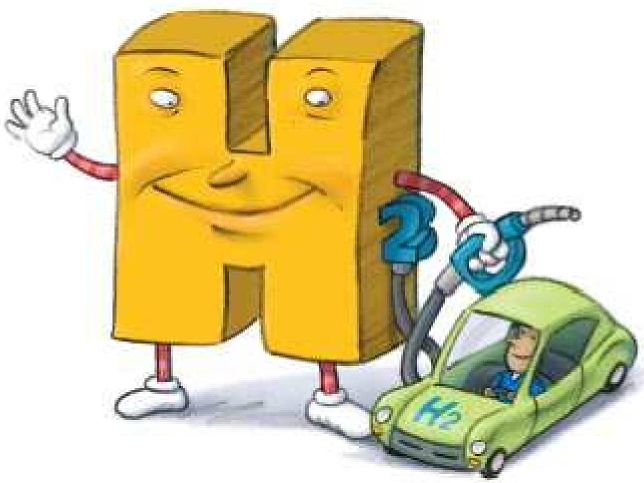
Conclusions

- Rayleigh-Taylor instability identified as credible combustion enhancing mechanism for the considered experiments.
- Following introduction of RT instability model into UU LES deflagration model, equation describing turbulent burning velocity recast as:

$$S_t = \left(S_u \times \Xi_k \times \Xi_{lp} \times \Xi_f \times \Xi_{RT}\right)\exp\left(u'/S_t\right)^2$$

- RT model implemented as an additional transport equation.
- In experimental scenarios investigated, introduction of RT model led to improvement of simulation results.
- Two user defined parameters contained in RT model: k_h & α:
  - α set as a constant throughout the calculation domain.
  - k_h set to 0.5 & 0.75 in area of external deflagration.

Thank you for your attention



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  - α set as a constant throughout the calculation domain.
  - k_h set to 0.5 & 0.75 in area of external deflagration.

Notes:

LES model (1/3)

- **Conservation of mass**

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\right) = 0$$

- **Conservation of momentum**

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{u}_i\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right) + \bar{\rho} g_i$$

- **Conservation of energy**

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{E}\right) + \frac{\partial}{\partial x_j}\left(\tilde{u}_j\left(\bar{\rho}\tilde{E} + \bar{p}\right)\right) =$$

$$= \frac{\partial}{\partial x_j}\left(\frac{\mu_{eff} c_p}{\mathrm{Pr}_{eff}}\frac{\partial \tilde{T}}{\partial x_j} - \sum_m \tilde{h}_m\left(-\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{Y}_m}{\partial x_j}\right) + \tilde{u}_i\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right) + \overline{S_c} \cdot H_c$$

LES model (2/3)

- Premixed flame front propagation (progress variable)

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{c}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial\tilde{c}}{\partial x_j}\right)+\overline{S}_c$$

- Gradient method for the source term

$$\overline{S_c}=\rho_u S_t\left\|\overrightarrow{grad}\left(\tilde{c}\right)\right\|$$

- The SGS turbulent combustion model for LES is based on the interaction of four mechanisms responsible for increase the flame front surface area:
  - Flow turbulence
  - Turbulence generated by the flame front itself
  - Preferential diffusion of stretched flame
  - Fractal-like flame wrinkling

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Existing UU turbulent burning velocity model

- Solves the conservation equations: mass, momentum and energy.
- Premixed flame front propagation, progress variable:
- Using gradient method for source term:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{c}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{c}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{c}}{\partial x_j}\right)+\bar{S}_c \quad , \quad \bar{S}_c=\rho_u S_t\left\|\overrightarrow{grad}(\tilde{c})\right\|$$

- Existing multi-phenomena turbulent burning velocity model for LES of premixed combustion is defined by:
  - Flow turbulence
  - Turbulence generated by the flame front itself (TGFF)
  - Preferential diffusion of stretched flame
  - Fractal-like flame wrinkling

$$S_t=[S_u\cdot\Xi_K\cdot\Xi_{lp}\cdot\Xi_f]\cdot\exp(u'/S_t)^2$$

Flow Turbulence

- Renormalization group (RNG) theory is the basis of the developed LES model
- Yakhot et al 1986, S_u substituted with S_t^{SGS}

$$S_t = S_u \exp\left(\frac{u'}{S_t}\right)^2 \quad \Rightarrow \quad S_t = S_t^{SGS} \exp\left(\frac{u'}{S_t}\right)^2$$

- Renormalisation group (RNG) SGS turbulence viscous model

$$\mu_{eff} = \mu\left[1 + H\left(\frac{\mu_s^2 \mu_{eff}}{\mu^3} - 100\right)\right]^{1/3}$$

$$\mu_s = \bar{\rho}\left(0.157 V_{CV}^{1/3}\right)^2 \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- In highly turbulent flows

$$\mu_{eff} = \mu_s \qquad u'_{sgs} = \sqrt{\frac{2}{3}\frac{\mu_t}{\rho\left(0.157 V_{CV}^{1/3}\right)}}$$

Turbulence Generated by the flame front itself

- Karlovitz (1951)
- Upper limit of flame-induced turbulence: $$u' = \frac{(E_i - 1) \cdot S_u}{\sqrt{3}}$$
- Upper limit for the flame-generated turbulence factor:

$$\Xi_K^{\max} = \frac{S_t}{S_u} = \frac{(E_i - 1)}{\sqrt{3}}$$

- Gostinstev et al 1989 reported transition from laminar to fully developed turbulent regime at R_0=1-1.2m for near Stoichiometric H_2-air.
- Formula applied in the SGS for transient value of flame wrinkling factor:

$$\Xi_K = 1 + \left(\psi \cdot \Xi_K^{\max} - 1\right) \cdot \left[1 - \exp\left(-R / R*\right)\right]$$

$R =$ Distance from ignition source

$\psi < 1 =$ Empirical coefficient

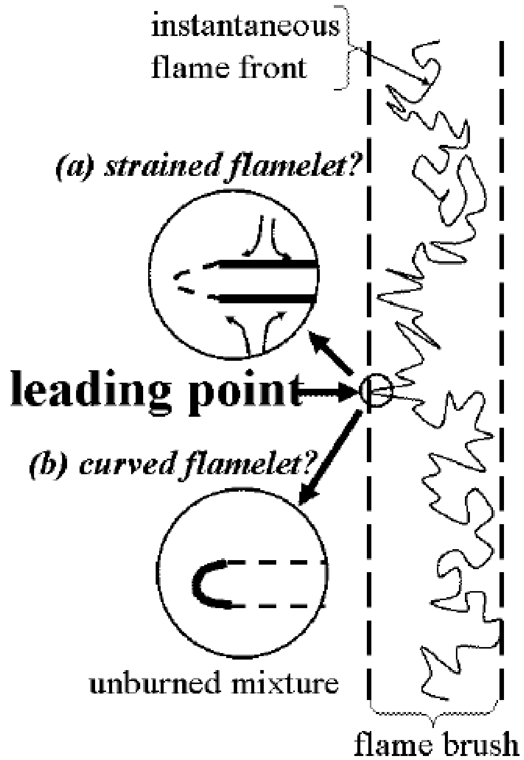
Preferential diffusion

- Kuznetsov and Sabelnikov, 1990
- Turbulent flame speed is led by the reaction zone areas most protruded into the unburnt mixture.
- Mixture composition locally altered by differences in diffusivities of fuel and oxidiser.
- Within the leading point combustion zone:

$$\alpha_{lp} = \frac{\alpha_0 (1 + C_{st}) \cdot d + d - 1}{d + C_{st}}, \alpha_{lp} \geq 1$$

$$\alpha_{lp} = \frac{\alpha_0 (C_{st} + d)}{1 + \alpha_0 \cdot C_{st} + C_{st} \cdot (1 - \alpha_0 \cdot d)}, \alpha_{lp} \leq 1$$

$$d = \left(\frac{D_{ox}}{D_f} \right)^{0.5} \qquad \alpha = \frac{1}{\phi}$$



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Fractal-like flame wrinkling

- Used to describe highly contorted, roughened curves and surfaces.
- The flame surface area of outward propagating turbulent flames will grow as $R^2.R^{D-2}$, where D is the fractal dimension (2.11-2.35).
- The integral scale of the problem R is the outer cut-off.
- The inner cut-off is chosen as a laminar flame front thickness: $\varepsilon \approx \delta_L$
- The effect of changing temperature of unburned mixture and explosion pressure on the inner cut-off:

$$\delta_L = \nu / S_u \qquad \nu = \text{ kinematic viscosity}$$

- To exclude a stage of quasi-laminar / transitional flame propagation after ignition up to the critical radius $R*$: additional wrinkling coefficient due to the fractals nature of turbulent premixed flame to be applied after $R*$ is:

$$\Xi_f = \left(\frac{R \cdot \varepsilon_{R*}}{R * \cdot \varepsilon} \right)^{D-2} \quad \text{with} \quad D = \frac{2.05}{u'/S_u + 1} + \frac{2.35}{S_u/u' + 1}$$

(North & Santavicca 1990)

Leading point factor

- Using the formulation by Kuznetsov and Sabelnikov, Zimont and Lipatnikov determined the hydrogen concentration at the leading points and found corresponding values of burning velocities by linear interpolation of the experimental data provided by Karpov and Severin.