A Dynamic Sub-grid Scale Model for LES of Deflagrating Flames

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Outline of the Presentation

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- Why LES ?
- Sub-grid Scale (SGS) Reaction Rate Models
  - Simple Algebraic Model
  - Dynamic Model
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Objectives

- To develop and test a dynamic sub-grid scale (SGS) model for chemical reaction rate.
- Numerical Implementation of the dynamic SGS model.
- Accounting the un-resolved SGS reaction rate contributions.
- Studying the effect of turbulence level and length scales on burning rates.
- Identifying the interactions between flame front and the flow field.

Why LES ?

- The unique feature of LES is filtering the scales in the exact solution into two categories; (i) Resolved (ii) SGS.

- Resolved scales or large eddies are computed explicitly and the SGS or small eddies are modelled.

- Accuracy of the solution – (a) Percentage of the energy
  (b) Sub-grid scale models

- Affordable computational times.

- In between RANS and DNS.

Governing Equations

- Mass Conservation

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_j)}{\partial x_j}=0$$

- Momentum Conservation

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_j}=-\frac{\partial P}{\partial x_i}+\frac{\partial \sigma_{ij}}{\partial x_j}$$

- Energy Equation

$$\frac{\partial(\rho h)}{\partial t}+\frac{\partial(\rho u_j h)}{\partial x_j}=\frac{\partial P}{\partial t}+\sigma_{ij}\frac{\partial u_j}{\partial x_i}-\frac{\partial q_j}{\partial x_j}+q_c$$

- Reaction Progress Variable Equation

$$\frac{\partial \rho c}{\partial t}+\frac{\partial\left(\rho u_j c\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Sc}}\frac{\partial c}{\partial x_j}\right)+\dot{\omega}_c \qquad \text{where } c=1-\frac{Y_{fu}}{Y_{fu}^{o}}$$

- State Equation

$$P=\rho RT$$

Reaction Rate Models (1/3)

(A) Simple Algebraic Model:

Based on flame surface density concept

Reaction rate is defined as $\bar{\dot{\omega}}_c = \rho_u u_L \bar{\Sigma}$

where as ρ_u is the density of un-burned mixture,

u_L is the laminar flame speed and

Σ is the flame surface density

Over bar indicates filtering operation

$$\bar{\Sigma} = 4\beta \frac{\tilde{c}(1-\tilde{c})}{\bar{\Delta}}$$

Reaction Rate Models (2/3)

(B) Dynamic SGS model :

Objective of the dynamic model is to identify the un-resolved flame surface density contribution and to account them.

The Flame surface density $\overline{\Sigma} = |\overline{\nabla c}|$ is the main term to be model.

$$\overline{\Sigma} = \left|\overline{\nabla c}\right| = \underbrace{\Pi\left(\overline{c},\overline{\Delta}\right)}_{\text{Resolved}} + \underbrace{\left(\left|\overline{\nabla c}\right| - \Pi\left(\overline{c},\overline{\Delta}\right)\right)}_{\text{Unresolved}}$$

Following similarity ideas of Germano and assuming sub-grid scale contribution of unresolved FSD at test filter, we can write dynamic SGS equation as

$$\overline{\Sigma} = \Pi\left(\overline{c},\overline{\Delta}\right) + K_s\left[\widehat{\Pi\left(\overline{c},\overline{\Delta}\right)} - \Pi\left(\hat{\overline{c}},\hat{\overline{\Delta}}\right)\right]$$

Reaction Rate Models (3/3)

K_s is the model coefficient, which can be dynamically calculated by identifying sub-grid scale flame surface as a fractal surface.

$$Ks = \frac{1}{1-\gamma^{2-D}}\left[\left(\frac{\bar{\Delta}}{\delta_c}\right)^{D-2} - 1\right]$$

where γ is the ratio of test filter to grid filter,

D is the fractal dimension and

δ_c is the lower cut-off length.

Dynamic model for *D:*

$$D = \frac{2.19}{\left(\frac{u'_\Delta}{u_L}+1\right)} + \frac{2.35}{\left(\frac{u_L}{u'_\Delta}+1\right)}$$

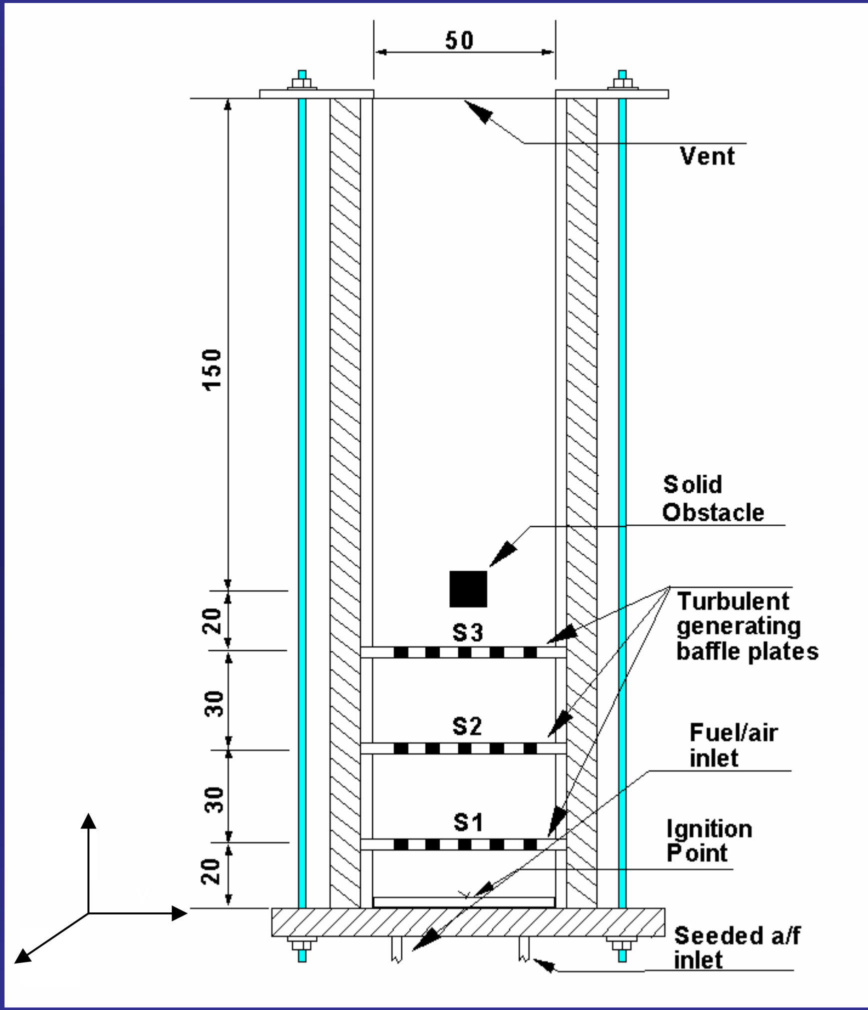
Model I

$$D = 2 + \frac{\log\left(\left\langle \widehat{\Pi(\bar{c},\bar{\Delta})}\right\rangle \Big/ \left\langle \Pi(\hat{\bar{c}},\hat{\bar{\Delta}})\right\rangle\right)}{\log\gamma}$$

Model II

Experimental Test Case (1/2)

- 50 x 50 mm cross-section
- 250 mm length
- 0.625 Liters
- Dual Assembly System
  - Inner assembly secures turbulence inducing obstacles
  - Outer assembly encapsulates inner assembly
- Held together by draw bolts
- Fuel: LPG (88% C_3H_8 , 10% C_3H_6)



Experimental Test Case (2/2)

Obstacle Geometry

- 1x Square Obstacle 12x12 mm cross-section
- Up to 3x Turbulence Generating grids (baffles)
- Aluminum baffles of 5 x 4mm Strips rending a blockage of ration of 40%.

Computational Domain

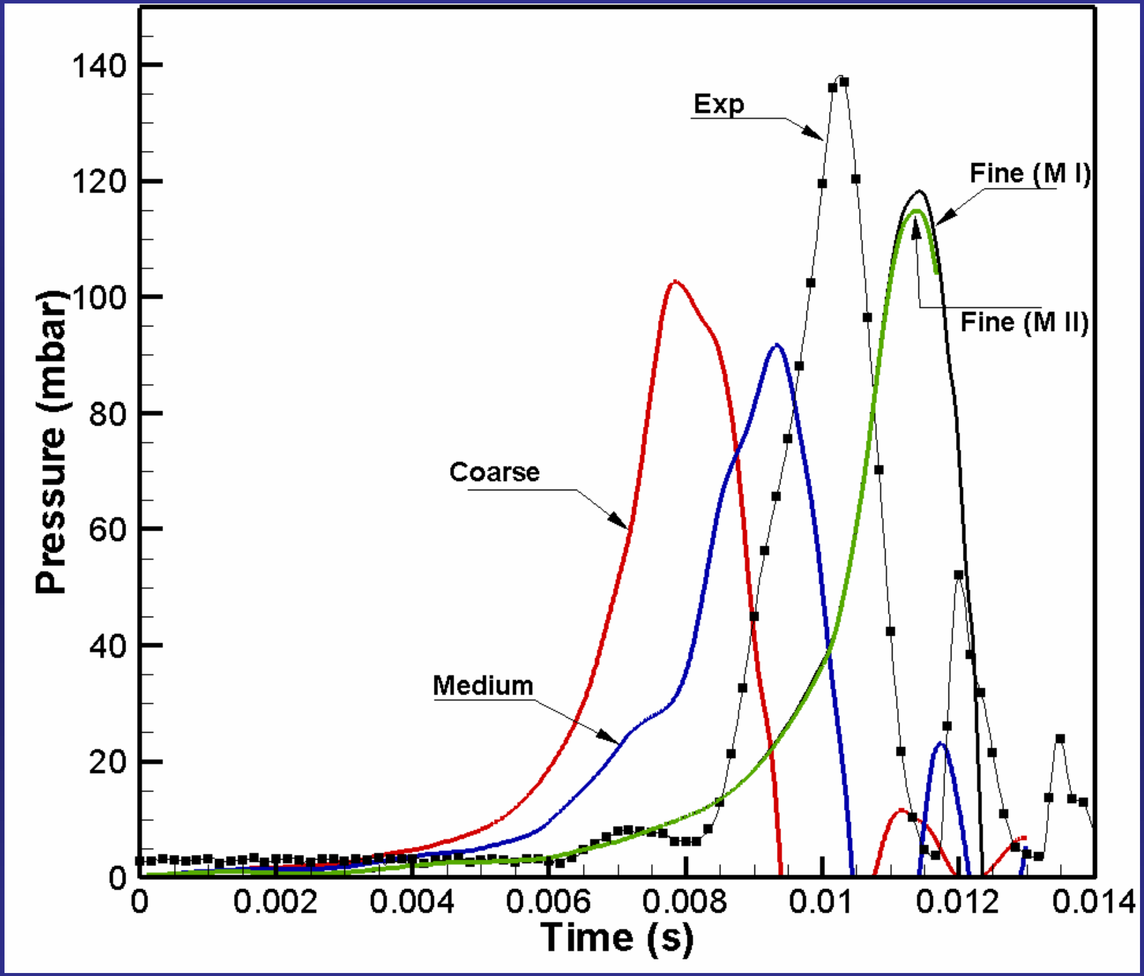
- 3-D, non-uniform Cartesian co-ordinate system.
- Chamber is of 50 x 50 x 250 mm and is extended to 325 mm in x, y and 250 mm in z direction with the far-field boundary conditions .
- 3 grids of 0.25, 0.55 and 2.7 million resolution.
- Solid boundary conditions are applied at walls, baffles and obstacle, with the power-law wall function.
- Out-flow boundary condition at the top of domain.
- The initial conditions are quiescent with zero velocity and reaction progress variable.

Results (1/7)

Key Findings:

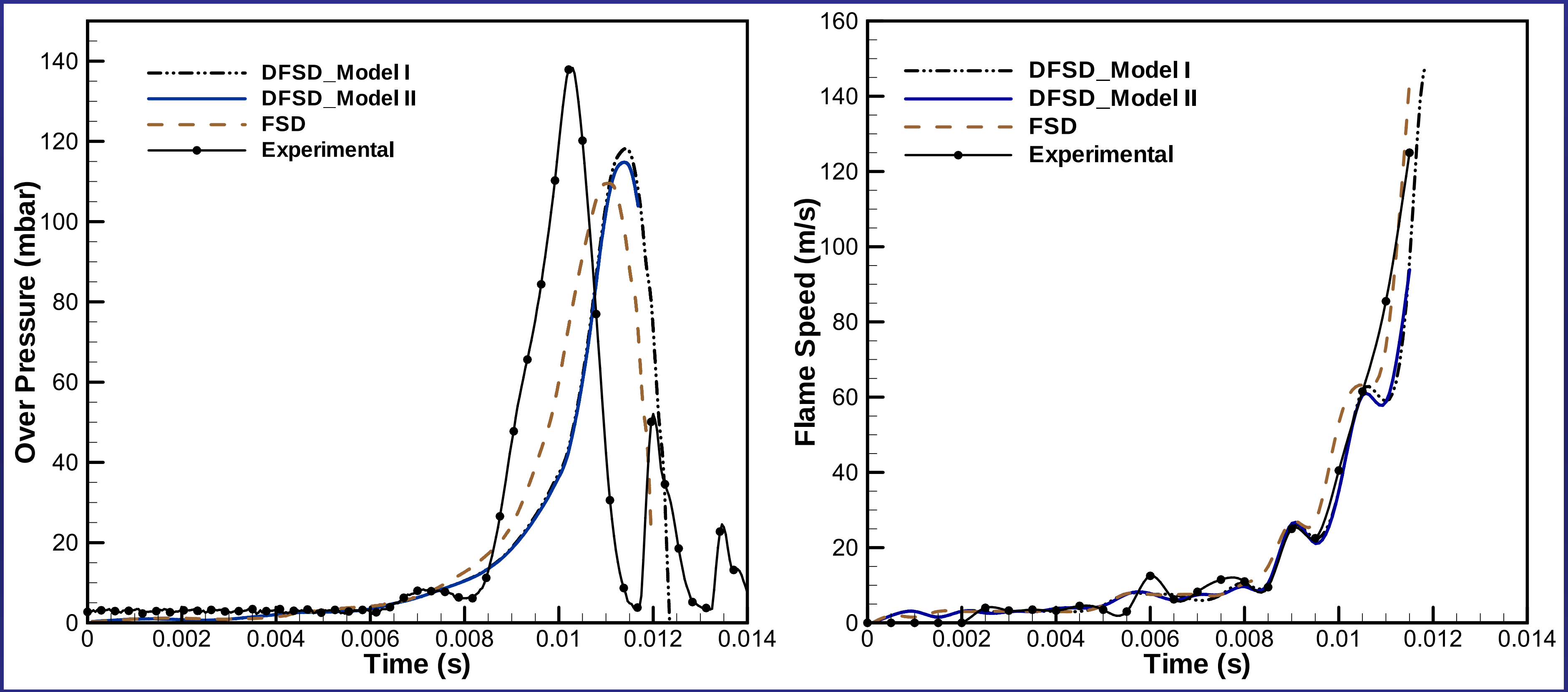
- Fine grid results are in good comparison with experimental measurements.
- Additional reaction rate due to the unresolved flame surface density is successfully captured.
- Both the models for fractal dimension has predicted the fractal dimension well.
- The dynamic model is able to predict overall flame structure, speed and propagating mechanism.

Results (2/7)



Time traces of the over pressure from LES of dynamic SGS model and experimental measurements

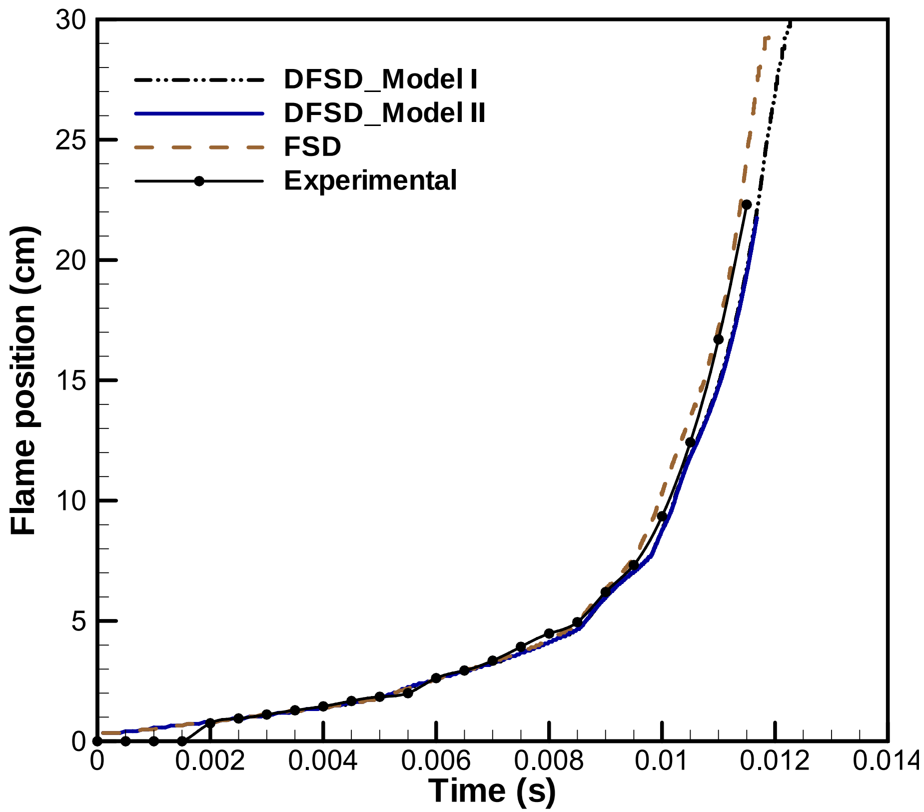
Results (3/7)



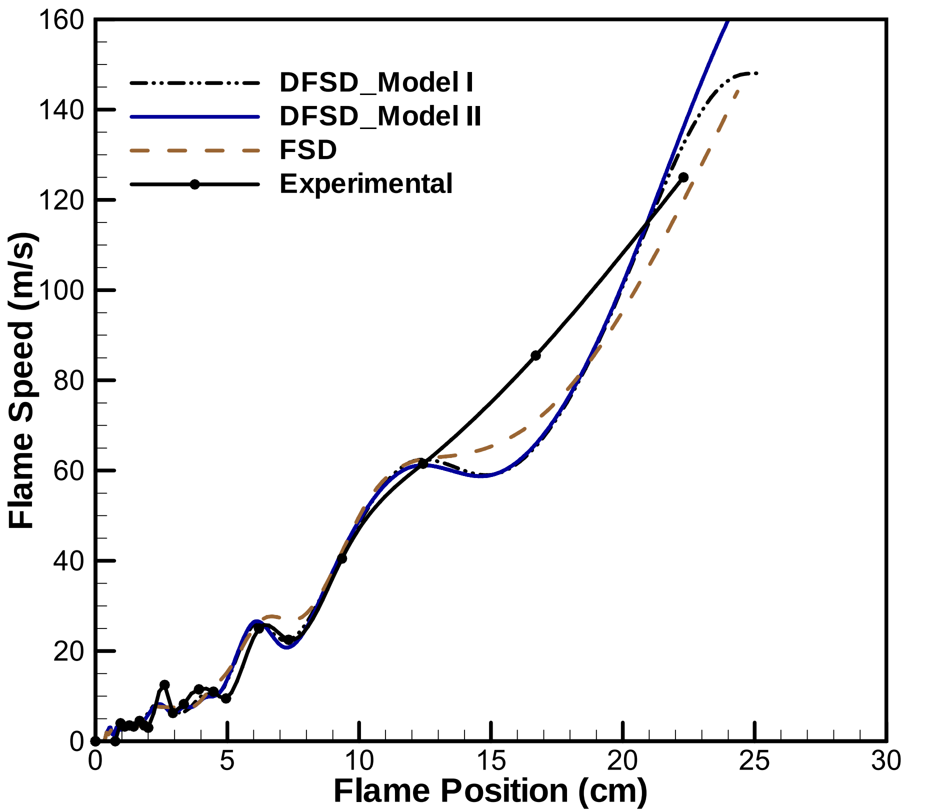
Time traces of Peak over pressure

Time traces of Flame speed

Results (4/7)

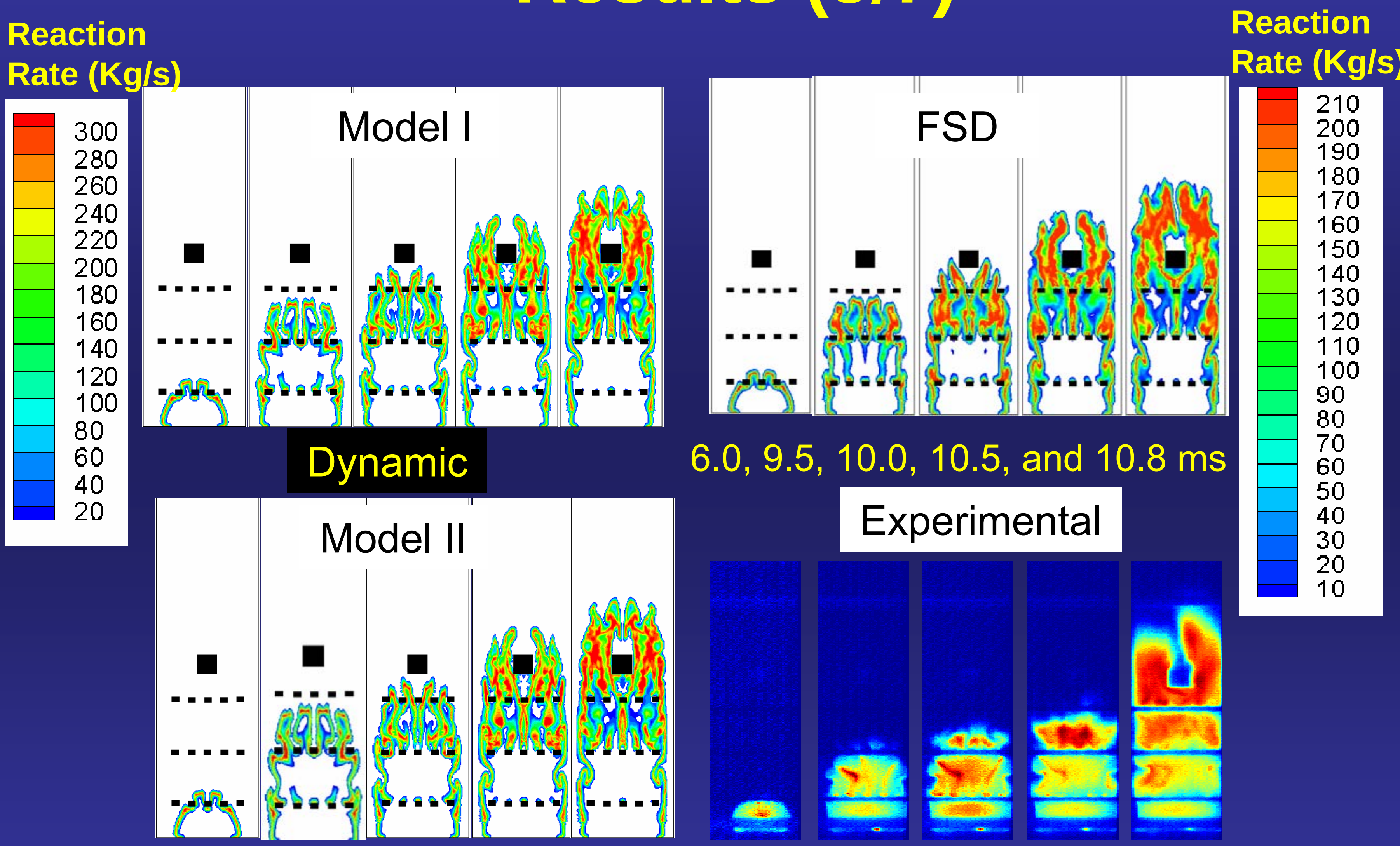


Time traces of Flame position



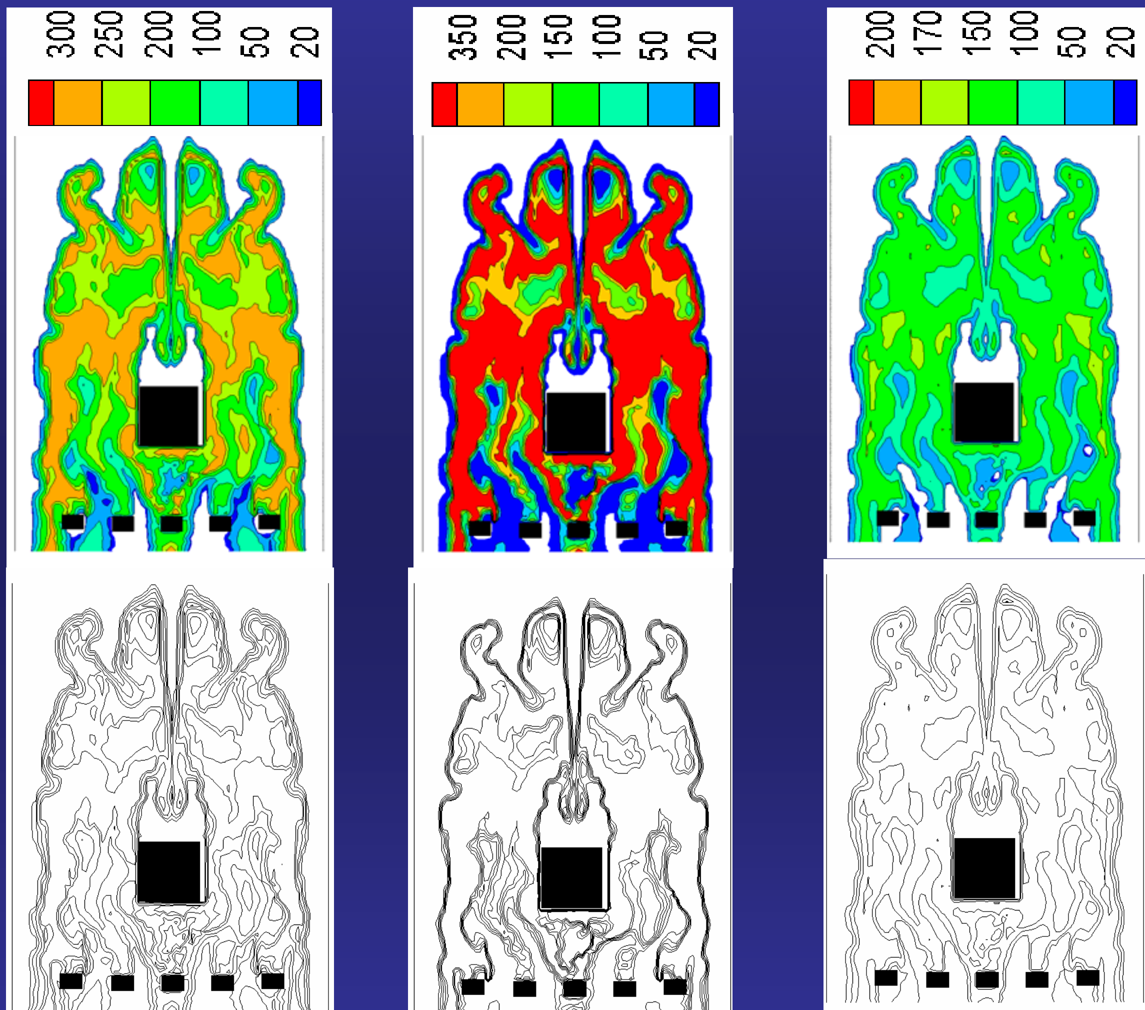
Flame position vs. Speed

Results (5/7)



Sequence of images to show flame structure at different times after ignition.

Results (6/7)



Reaction rate Kg/s

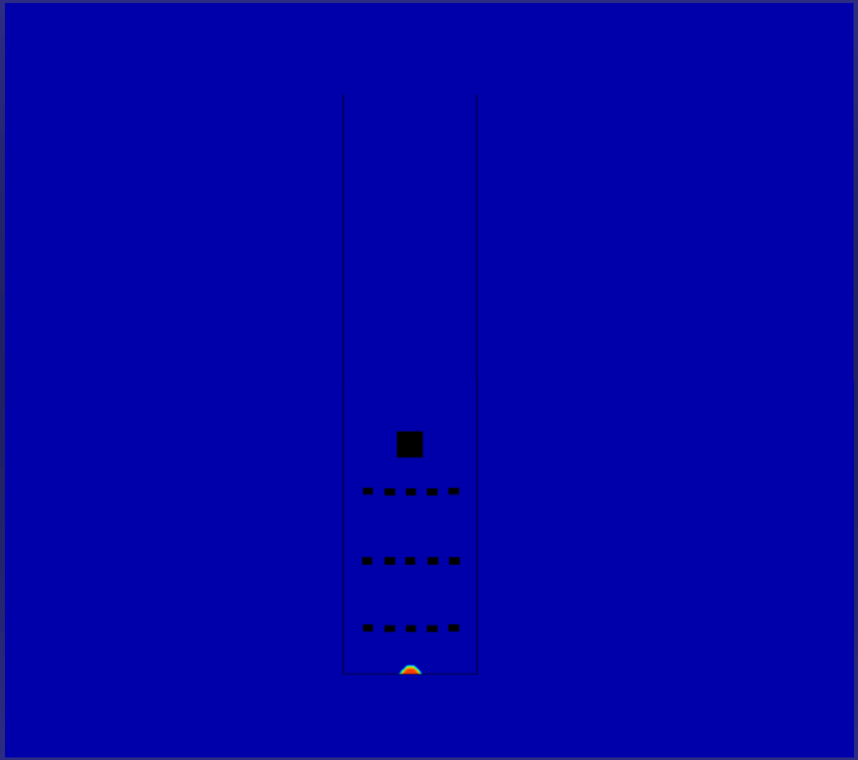
Resolved contributions

Un-resolved contributions

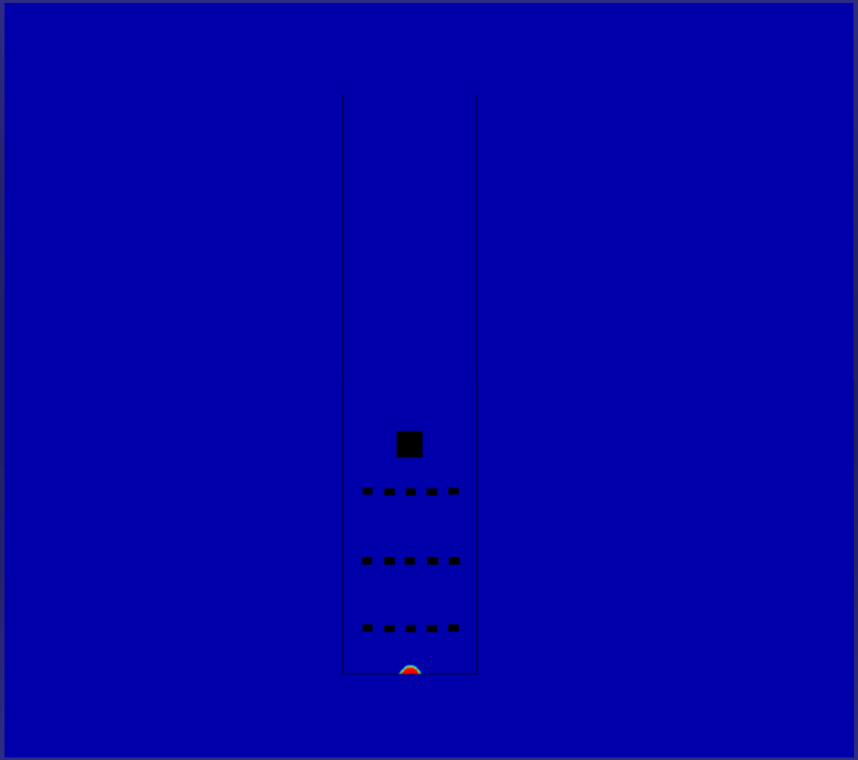
Flame after 11.0 ms of the ignition using dynamic sub-grid scale model.

Results (7/7)

Reaction rate



Dynamic sub-grid scale model



Simple algebraic model

Conclusions

- LES simulations were carried for turbulent premixed deflagrating flame using two models for reaction rate, namely a novel dynamic sub-grid scale model and the conventional FSD models.
- The new dynamic model is implemented, tested and results are compared with the experimental measurements.
- The dynamic model has remarkably predicted the contributions of unresolved SGS reaction rate and the overall features of the turbulent propagating flame.
- Fractal dimension is calculated using an empirical and a dynamic model. Both the models predicted the turbulent premixed flames successfully.
- Overall, the LES simulations with dynamic model are very encouraging to simulate more complex premixed flames.

Further Work

- Identifying the proper model for lower cut-off length.
- Studying other flow configurations using dynamic model.
- Parametric analysis of the model in terms of the present explosion chamber.
- Identifying the possibilities to extend this model for detailed chemistry problems.