# Predicting Flame Acceleration Using a Coherent Flame Model

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## 1 Introduction

Flame acceleration is needed for the development of slow combustion front generating little overpressure to a severe gas explosion with a fast moving flame. A comprehensive review of the considerable volume of the work on this topic was recently given by Ciccarelli and Dorofeev [1] with emphasis placed on experimental investigation. It is well established through past experimental investigations that the presence of the obstacles would greatly increase flame speeds, overpressures, and could at high flame velocities a tendency for deflagration to detonation transition (DDT) compared to similar tests without obstacles. It was believed that turbulence in the unburned gas and the obstacles provide a powerful means of transferring mean flow kinetic energy into turbulent kinetic energy: Interaction of the flame with the obstacles promotes strong mixing and hence rapid combustion in the turbulent flame zone. Despite various attempt to numerically predict the dynamic three-way dynamic interaction of flame, turbulence and obstacles, there still lacks a robust code which can capture in detail this complex phenomena with accuracy.

In the present study, a coherent flame model has been implemented into the large eddy simulation (LES) frame of the OPENFOAM code. Predictions are made between the predictions and the experimental data firstly for a spherical flame [3] and then a rectangular shock tube [4]. The reasonably good agreement achieved demonstrates the potential for the model to be further developed and extended towards predicting DDT.

## 2 Mathematical Formulation

The LES solver of the CFD code OPENFOAM is used. The OpenFOAM (Open Field Operation and Manipulation) CFD Toolbox can simulate complex fluid flows involving chemical reactions, turbulence heat transfer. OpenFOAM uses finite volume numerics to solve systems of partial differential equations ascribed on any 3D unstructured mesh of polyhedral cells. The fluid flow solvers are developed within a robust, implicit, pressure-velocity, iterative solution framework, although alternative techniques are applied to other continuum mechanics solvers. The code, produced by OpenCFD Ltd, is open-source and available freely the GNU General Public Licence.

Previous premixed combustion modelling approaches in LES have been mainly based on the artificial thickening of a flame or on the “G-equation”, which was considered as only valid on the flame surface and suffers from significant drawbacks. The laminar flamelet approach appears as an interesting alternative according to the combustion diagram from Borghi and considering typical Damköhler and Karlovitz numbers of about Da ~ 10–100 and Ka ~ 0.01–1. Algebraic

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models have already been proposed for the flame surface density (FSD) in LES applications. Balance equations for the wrinkling factor or the FSD have also been investigated. For flame acceleration around obstacles, the correct description of the wrinkling evolution is crucial, giving an advantage to the balance equation formulation. Within the OPENFOAM code, there is already a two equation turbulent deflagration model which solves the wrinkling factor equation and regress variable transport equation. The major drawback of this model within the LES context is the lack of sub-grid contribution. We have hence decided to adopt the coherent flame model recently developed by Veynante and co-workers [2], which combines an Eulerian spark ignition model derived from the RANS AKTIM model and a Coherent Flame Model (CFM) describing the flame propagation.

## 3 Results

Predictions are firstly made for the experimental case of Renou and Boukhalfa [3]. A propane–air mixture is injected through a turbulence grid into a channel where a thin spark plug ignited the mixture. The turbulence was found to be nearly isotropic (PIV and laser tomography imaging) and hardly decayed during the flame kernel growth.

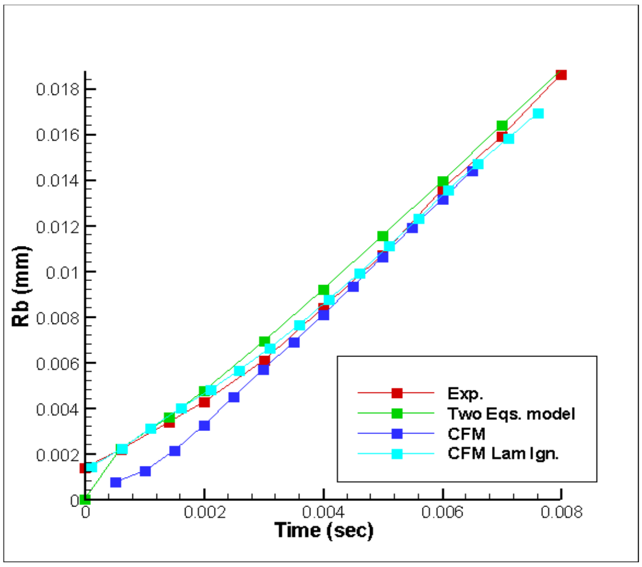


Figure 1 Evolution of the mean flame radii – comparison between the predictions of different models and experiment data in [3].

In Figure 1, comparison is made between the measurements of Renou and Boukhalfa [3] and the predictions from the original two equation model deflagration model in OPENFOAM and the coherent flame model of Richard et al. [2] which has been newly implemented. In this simple case, both models are found to be in reasonably good agreement with the data apart from the initial stage. As the flame is initially laminar in this case, it was found necessary to retain a model evolution equation for the spark wrinkling equation and define a local FSD. The predictions with the modification are shown in Figure 1 as “CFM Lam Ign” and are found to be in very good agreement with the data.

The $2^{nd}$ case considered is the experiments of Patel et al. [4] for deflagration in a semi-confined explosion chamber. Laser diagnostics techniques were used to investigate flame propagation past multiple obstacles mounted in the chamber. Pressure was measured at two locations within the combustion chamber. The computational domain, as shown in Figure 2, is 150 x 150 x 500 mm with average mesh size of 2mm. This gave a maximum Courant number of 0.2. The domain consists of 0.5M grid cells in total and as shown in Figure 2, the domain is extended both vertically and horizontally beyond the opening of the chamber. The stoichiometric methane and air mixture has an initial temperature of 300K and pressure of 1 bar.

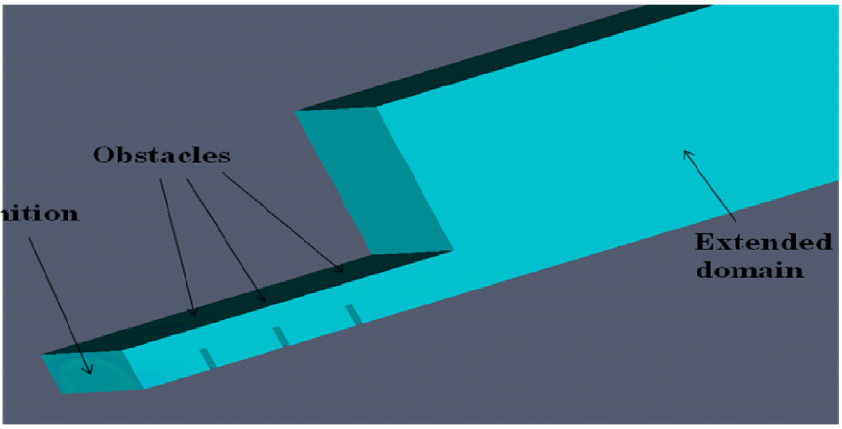


Figure 2 Computational domain for the explosion chamber

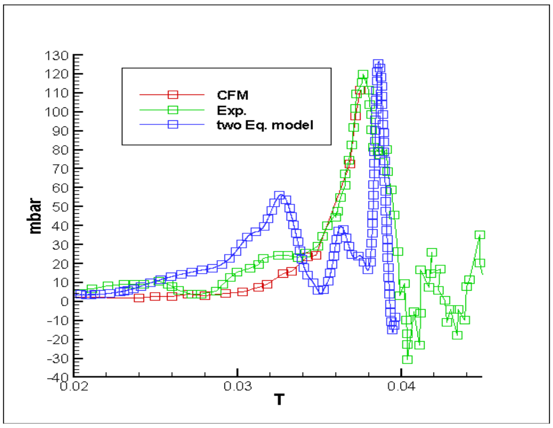


Figure 3 Comparison between predicted and measured overpressure

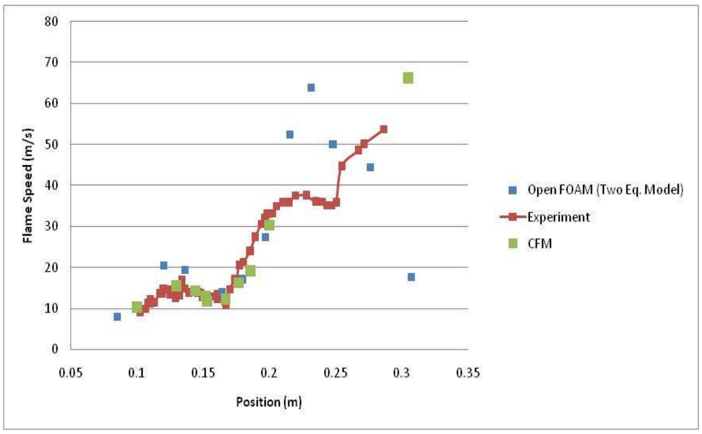
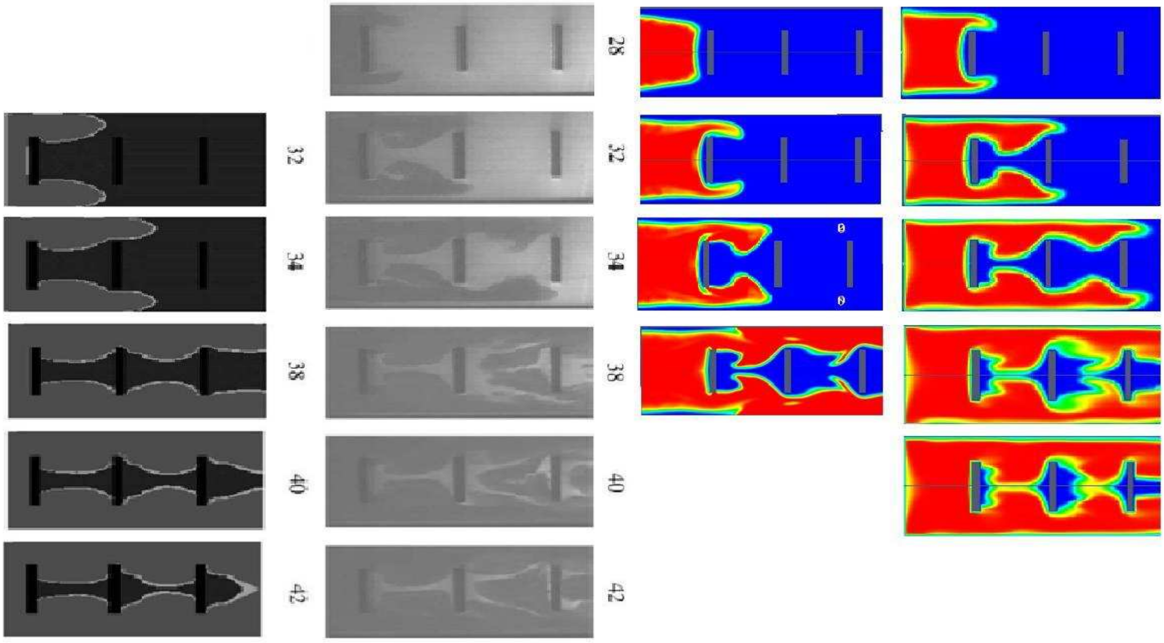


Figure 4 Comparison between predicted and measured flame front speed values at different locations from the ignition end

In Figures 3, comparison is made between between the predicted and measured overpressure at different times. The coherent flame model has demonstrated considerable improvement over the original two equation turbulent deflagration model in OPENFOAM. Even more encouraging agreement is seen in Figure 4 when comparison is made between the predicted and measured flame front speed at different locations from the ignition end.

In Figure 5, comparison is made between the present predictions using both the CFM modified OPENFOAM and the original code with the two equation turbulent deflagration model with the measurement and RANS simulations of Patel et al. [4]. It can be seen that the predictions with CFM shows an evolution pattern which more closely resembles the experimental measurement.



RANS simulation [4] Experiment [4] CFM OPENFOAM two eq. model

Figure 5: Flame evolution – comparison between the present predictions with the measurement and RANS simulations of Patel et al. [4]

## 4. Conclusion

A Coherent Flame Model (CFM) has been implemented in OpenFOAM. The implementation has also included the spark ignition model AKTIM (Arc and Kernel Tracking Ignition Model) and Artificial burning progress. Preliminary results indicated that the model predicted with reasonable accuracy spherical flame propagation from a stoichiometric propane-air mixture and it delivers improved predictions for flame acceleration in a rectangular shock tube with obstacles.

## References

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