THE APPLICATION OF A LAMINAR FLAMELET MODEL TO CONFINED EXPLOSION HAZARDS

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The release of a flammable vapour into the atmosphere and its subsequent ignition can lead to a fast-moving deflagration wave which, in the presence of adequate confinement and obstacles, can result in high overpressures. The need to be able to model such situations is increasingly important in order to aid the design and hazard assessment of many structures, such as process plants and offshore platforms in the oil and gas industries. Recently, considerable efforts have been made to improve both the available experimental data and modelling techniques. However, these have highlighted the lack of knowledge in this area and the inaccuracy of many of the current modelling techniques, which is due to both the low resolution meshes that are often required in order to attain reasonable computational times for the complex geometries involved and to a lack of understanding of the physics, in particular the turbulence/combustion interaction.

In order to resolve accurately the shear layers around obstacles, approximately 10 cells are required across the thickness of the shear layer [1]. Within the constraints of the currently available computing power, structured meshes are limited to geometries with order 10 obstacles. The pragmatic approach to computing larger geometries has been to use porosity distributed resistance (PDR) models [2]. Here obstacles are not resolved, but are represented by additional resistance terms appended to the transport equations. Such methods are limited by the accuracy of the resistance terms, which can only be improved by access to extensive and very expensive experimental data or data from high quality resolved computations.

The aim of the present work is to develop a methodology capable of handling efficiently complex geometries and combining this with the best available modelling, in order to perform resolved computations for explosions with order hundred obstacles.

The majority of numerical models applied to confined explosion hazards employ the Eddy Break-up (EBU) [e.g. 3] combustion model, in various forms, due to its simplicity and it very low computational expense. This model is known to have a number of serious deficiencies, such as insensitivity to mixture composition and fuel type, inability to predict correct burning rate near walls, and difficulty in the specification *a priori* of the model constant. Palliative techniques, such as leading edge quenching [4], are invariably applied to prevent unphysical effects and allow reasonably realistic flame shapes to be predicted. However, such measures are undesirable since they remove important aspects of the physics from the calculations. Better combustion models are available, but these have not yet been widely applied to practical problems involving complex geometries. The laminar flamelet model [5, 6] is now well established as being able to model accurately many combustion applications of practical interest and this work applies a computationally efficient laminar flamelet model to confined explosion hazards.

Laminar flamelet models assume that all reaction takes place in thin, highly wrinkled surfaces that separate unburned reactants from fully-burned products. These surfaces are stretched and transported by the turbulence, but retain the local structure of strained laminar flames, whose reaction rate can be evaluated using, for example, one-dimensional counterflow laminar flames [7]. In the laminar flamelet limit the mean turbulent reaction rate is viewed as the product of the mean reaction rate per unit surface area (R) and the mean flame surface area per unit volume $(\overline{\Sigma})$.

Various methods have been proposed for calculating $\overline{\Sigma}$. The most rigorous of these involves the solution of an exact transport equation [8]. However, because of the considerable uncertainties in the modelling of the unclosed terms and the increased computational expense, an approach employing an algebraic relationship for $\overline{\Sigma}$ is applied here. The expression for $\overline{\Sigma}$ is obtained by treating the passage of laminar flamelets past a point as a stochastic process analogous to a random telegraph signal [9] and employing an empirical function [10] to correctly predict the behaviour near walls. The laminar flamespeed, required in order to calculate R, is calculated using an empirical correlation [10] eliminating the need for computational expensive flamelet libraries.

In modelling confined explosions an additional complexity arises from the necessity to model an initial laminar burning phase. After ignition, an initial flame kernel develops which propagates at the laminar flame speed. As the kernel grows, instabilities develop that cause the flame front to cusp and wrinkle, until transition to turbulent combustion occurs. The onset of this transition is accelerated by the turbulence generating properties of any obstacles that may be present. Although the highest overpressures are generated during the turbulent phase, it is essential to model accurately the laminar phase and particularly the transition. Rapid flame acceleration occurs during turbulent combustion, and increasing the duration of the laminar phase will decrease the proportion of the reaction that is turbulent and hence reduce the overpressures. Additionally, the flame arrival time is essentially dependent on the laminar burning rate and the point of transition. Without a treatment for the laminar flame phase overpressures are over predicted and flame arrival times are under predicted [11].

Ideally, for the laminar phase of the explosion a true laminar flame treatment could be used. However, it is impractical to resolve down to the laminar flame thickness, due to computational costs at least for a realistic geometry. Another possibility is to model the thickened laminar flame, resulting from the action of instabilities on the initial kernel. This approach requires the calculation of a term to represent the mean flame surface area per unit volume including the area enhancement due to flame wrinkling; at present such a term is not available and there is no available experimental data with which to devlop one. However, it is hoped that future results from direct numerical simulations will provide suitable data. The approach employed in the present work is a more pragmatic one. The laminar combustion model constrains the flame to burn at the laminar flame speed, by scaling the sum of the reaction rates at each node so that it is equal to the total reaction rate of a laminar flame with the same total flame surface area.

Central to the present approach is the geometric flexibility of an unstructured tetrahedral computational mesh [12]. This is combined with solution adaptive meshing to provide excellent computational efficiency. The confined explosion problem is an ideal application for adaptive meshing, since it is only close to the flame front that high spatial resolution is required. Away from the flame, a significantly lower resolution mesh can be employed without loss of accuracy. The mesh can refine and de-refine in both space and time such that it effectively follows the flame front. Refinement is applied on an arbitrary number of levels and a parent-child hierarchical structure is applied to the mesh storage, allowing rapid remeshing at regular intervals. Refinement criteria can be specified on any combination of variables**.** Turbulence closure is by means of a low Reynolds number k-ε model.

A number of test cases have been computed using the developed methodology. Initial calculations were two-dimensional in order to reduce computational expense during model development. Experimental data, in the form of the maximum peak overpressure, is available [13] for a series of channel test cases containing either baffles or centrally located obstacles. Figure 1 shows the reaction progress variable and the adapted mesh for an obstacle channel test case, 5.84ms after ignition. The initial mesh was coarse, containing only 929 nodes, but with adaptive mesh refinement to four levels, this increased to 21098 nodes by the time shown in the figure. To achieve an equivalent level of mesh resolution around the flame without adaptive refinement would require of the order of a million nodes and thus be too computationally expensive for practical use.

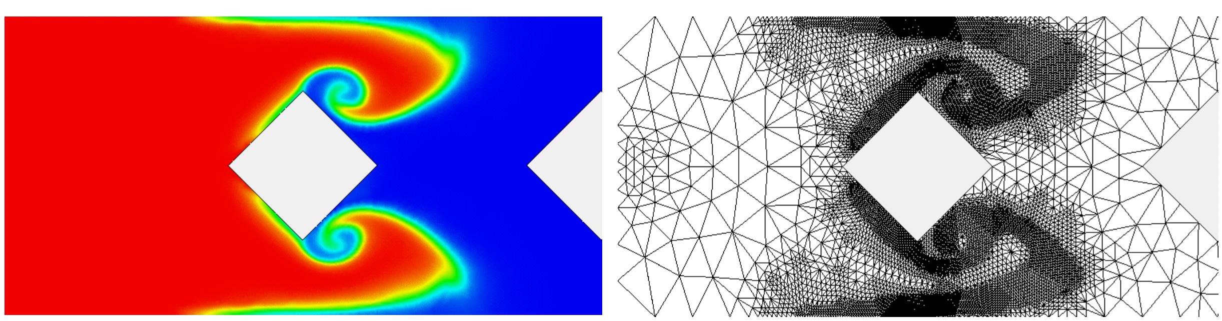

Figure 1. Reaction Progress Variable and Adapted Mesh for Obstacle Channel Test Case

Figure 2 shows the development of the reaction progress variable and adapted mesh for a baffled channel test case. As the flame propagates along the channel the mesh can be seen to follow the flame. As the flow accelerates past the baffles turbulence is generated increasing the flamespeed, whilst recirculation regions form behind the baffles into which the flame propagates more slowly. It is burning in the regions behind the baffles that is known to determine the maximum overpressure. The flameshapes shown compare very well with experimentally observed flameshapes [14]. However, such flameshapes were not predicted if a coarse mesh without adaptive mesh refinement was employed.

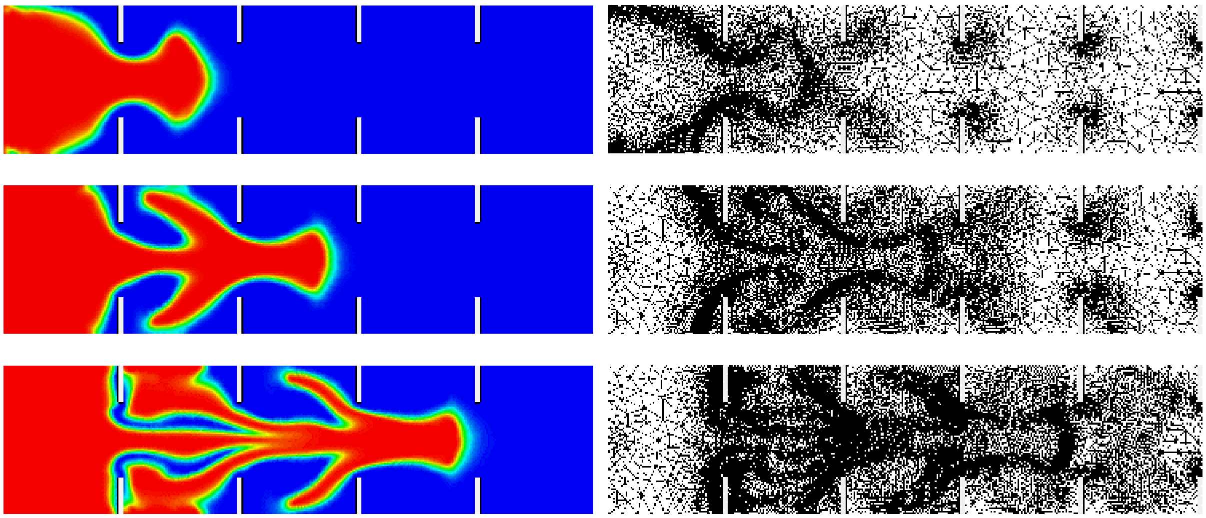

Figure 2. Reaction Progress Variable and Adapted Mesh for Baffled Channel Test Case

The principal effect of the laminar model is to slow down the initial flame development time and thus decrease the maximum overpressure. Flameshape predictions are not affected by the laminar phase. Table 1 compares the predicted overpressures with and without the laminar model for the two test cases shown in figures 1 and 2, with propane and methane as the fuel, to the experimental data [13]. Clearly, the inclusion of even a basic model for the initial laminar flame phase reduces the predicted overpressures significantly and improves the agreement with the experimental data.

Test case	Fuel	Experimental [13]	Predictions	
			Turbulent	Laminar & turbulent
Obstacle channel	10% CH_4	0.233	0.731	0.408
Baffled channel	10% CH_4	1.17	1.463	0.963
	4.5% C_3H_8	2.42	4.235	2.483

Table 1. Summary of Computational and Experimental Peak Overpressures (bar)

Figure 3 shows a snapshot of the reaction progress variable for a more realistic geometry, a slice through the Troll Wellhead geometry. This case demonstrates the ability to compute the flow around larger (284 obstacles), more complex geometries that could only previously computed using PDR methods. With extension to the available parallel computing capability, it will be possible to perform three-dimensional computations for such geometries and subsequently for real offshore modules.

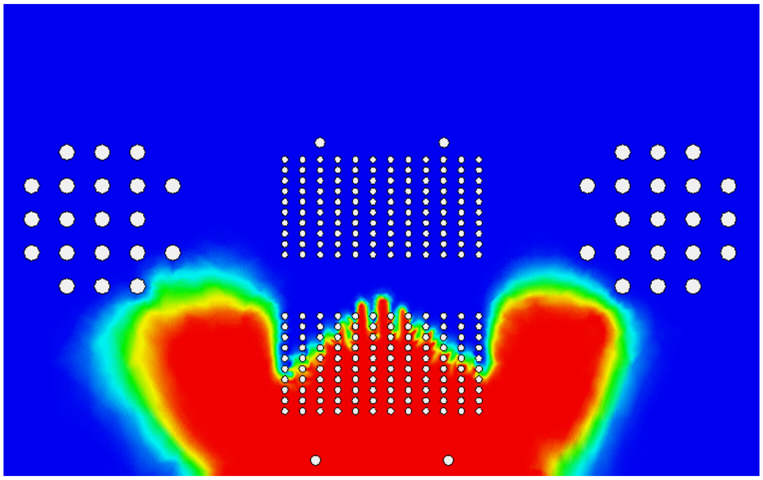

Figure 3. Reaction Progress Variable for the Troll Wellhead Geometry

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