

Predictions of the consequences of natural gas-hydrogen explosions using a novel CFD approach

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Abstract

There is increasing interest in the use of hydrogen as an energy carrier. A hydrogen delivery system is required, and one solution is its addition to existing natural gas pipeline networks. A major concern is the explosion hazard may be increased should an accidental release occur, and this paper presents results from the mathematical modelling of confined, vented explosions of mixtures of methane with 0%, 20% and 50% hydrogen dilution by volume. The flow field in an explosion was predicted through solution of the averaged forms of the Navier-Stokes equations, with these equations closed using both $k-\epsilon$ and second-moment turbulence models. Accurate representation of the turbulent burning velocity of the various mixtures was necessary, and this was achieved using correlations obtained from the analysis of extensive experimental data sets on H_2-CH_4 mixtures. Results, derived for explosions in a $70m^3$ confined vessel with and without pipe congestion, demonstrate that hydrogen addition can have a significant effect on overpressure generation, particularly if turbulence generating obstacles are present.

Keywords: CFD, deflagration, safety, hydrogen

1. Introduction

There is presently an increasing interest in the use of hydrogen as an energy carrier as an essential part of achieving a sustainable economic development. The work described was carried out as part of the NATURALHY project (see <http://www.naturalhy.net>), the main objective of which is to consider the potential for using the existing natural gas system as a means of transporting the hydrogen from a site of production to a point of use. Hydrogen would be transported in the gas network as a mixture and some hydrogen extracted for hydrogen powered applications. However, some hydrogen would remain mixed with natural gas and be delivered to existing gas customers where it would be burned as a mixture.

One major concern in this work is that the explosion hazard may be increased, as in contrast to natural gas, hydrogen has a relatively high burning velocity, and can easily make the transition from deflagration to detonation. It is therefore essential to investigate the possible behaviour of such gaseous mixture releases in both confined and unconfined areas of industrial relevance. Subsequently, the information obtained can be used in the design of equipment and plant, and to improve safety and reduce the risk of both deflagrations, and deflagration to detonation transitions.

This paper presents results from the mathematical modelling of confined, vented explosions with and without internal pipe-work congestion. The mixtures investigated comprised methane, used to represent natural gas, with 0%, 20% and 50% hydrogen dilution by volume. One objective of this study was the comparison of turbulence model performance, and the turbulent flow field was resolved by the application of both a two-equation and a second-moment turbulence closure, supplemented with transport equations for the reaction progress variable and the total energy. Accurate representation of the turbulent burning velocity of the various mixtures is necessary, and this was introduced into the calculation via the diffusion coefficient and the source term of the reaction progress variable. The burning velocity was represented by correlations obtained from the analysis of recent experimental data gathered at the University of Leeds, and a simple eddy break-up reaction model using a one-step irreversible reaction was applied in the prescription of the turbulent combustion model.

The calculations presented are representative of confined, vented explosion experiments undertaken by Loughborough University in a 70m³ confined vessel with and without internal pipe-work congestion. The results are conforming to experimental observation (Hankinson and Lowesmith, 2007), however a full experimental dataset remains in preparation and as such, is not reported in the present work. Future publication will provide full comparisons.

2. Experimental Arrangement

The predictions presented in this paper are a selection taken from a number of simulations of large-scale experiments undertaken by Loughborough University (Hankinson and Lowesmith, 2007). A full account of the experiments performed and the results obtained will be presented elsewhere, hence only a brief overview is given here. The experimental rig was of steel construction, and measured 8.25m in length, 3.0m in width, and 2.8m in height. One 3.0 × 2.8m end was effectively open to the atmosphere for the purpose of the tests, being covered with a polythene sheet to retain the gas-air mixture prior to ignition. Figure 1 depicts the rig, and indicates the configuration of pipe-work congestion and the spark ignition points, although not to scale.

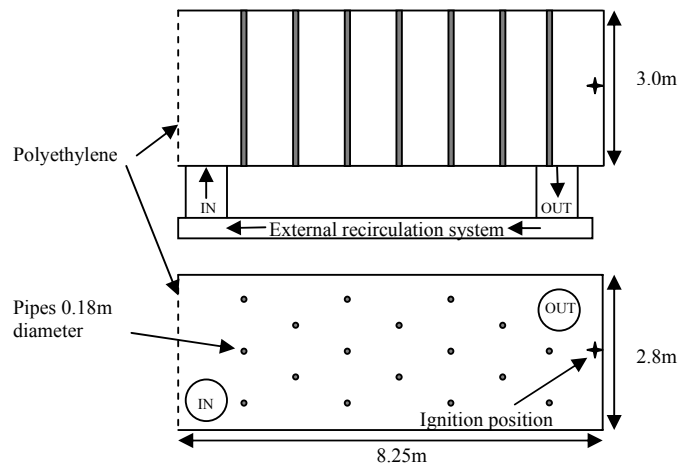


Figure 1. Schematic diagram of the experimental rig.

The gases investigated were mixtures of methane, hydrogen and air, with the methane-to-hydrogen ratio by volume being 100:0, 80:20 and 50:50. Five tests for computational investigation were chosen as a representative sample of the total number of experiments performed, and these configurations are reported in Table 1.

Table 1. Experimental conditions.

Experiment number	Fuel / CH ₄ :H ₂	Congestion / pipes	Ignition location
7	80:20	None	Rear
8	50:50	None	Rear
9	80:20	17	Rear
10	50:50	17	Rear
13	100:0	None	Rear

3. Mathematical Modelling

3.1. Turbulent Flow Field

The flow fields within the experimental rig were resolved by solution of the two- and three-dimensional forms of the density-weighted, partial differential equations describing the conservation of mass, momentum, and total energy. Time-dependent, and written in their high Reynolds number forms, the averaged equation set was closed in the first instance by the standard k-ε turbulence model of Jones and Launder (1972). Modelling constants used were the widely accepted standard values, as reported in Jones and Whitelaw (1982). For comparison, a second-moment method of turbulence closure was investigated, being that described by Jones and Musonge (1988). In this original aspect to the modelling approach, the shear and normal stress terms are closed by the solution of their individual transport equations, the modelling constants employed being a modified set, as described in Jones (1994).

The geometry was modelled using three approaches. In the first instance, a central section of that shown in Fig. 1, assuming symmetry properties of two of the computational boundaries, was used. Fig. 2 depicts this geometry, where the left boundary represents a solid wall, and the right an outflow. Initially, a small area of burned gas, represented by a region where the progress variable, c , equals 1.0, is located adjacent to the former boundary, which is used to instigate the numerical reaction. Secondly, a two-dimensional slice of the geometry was modelled using three solid wall boundaries, and containing a representation of all the specified obstacles. Thirdly, a full three-dimensional version of the confined region was modelled.

3.2. Combustion Model

In addition to that for total energy, E , the premixed combustion model implemented requires the solution of a conservation equation describing the reaction progress variable. The source term of this equation is represented by a modified form of the eddy break-up reaction rate expression as:

$$\overline{\rho S_c} = \bar{\rho} R \tilde{c}^4 (1 - \tilde{c}) \left(\frac{\rho_b}{\rho_u} \right) \quad (1)$$

where reactants are assumed to go to products in a single-step irreversible reaction, and a superscript bar and tilde represent, respectively, Reynolds and density-weighted

averaged mean values. Also, R represents the reaction rate established in line with discussion in Catlin et al. (1995), and ρ the densities of the burned and unburned gases indicated by the subscripts. This form of the reaction rate expression eliminates the cold-front quenching problem by prescribing variation of the reaction rate through the flame using a power law expression (Catlin et al., 1995). Equation (1) can be subsequently used in the closure of the source term for total internal energy by convolution with a representation of the specific heat release.

The two components of this model are to firstly provide solutions which give rise to a flame which accurately reproduces specified burning velocities, and secondly provide a representative prescription of these velocities given known mixture and flow field parameters. Following Catlin et al. (1995), the source terms and diffusion coefficients in the equations for E and c can be defined as functions of the turbulent burning velocity, and here, correlations derived from the most recent experimental evidence (see, for example, Burluka et al., 2007) have been implemented.

3.3. Method of Solution

Integration of the equations employed a second-order accurate finite-volume scheme in which the transport equations were discretised following a conservative control-volume approach, with values of the dependent variables being stored at the computational cell centres. Approximation of the diffusion and source terms was undertaken using central differencing, and a second-order accurate variant of Godunov's method applied with respect to the convective and pressure fluxes. The fully-explicit time-accurate method was a predictor-corrector procedure, where the predictor stage is spatially first-order, and used to provide an intermediate solution at the half-time between time-steps. This is then subsequently used at the corrector stage for the calculation of the second-order fluxes. A further explanation of this algorithm can be found elsewhere (Falle, 1991). An adaptive-grid method was employed to allow the generation of fine grids in regions of steep spatial and temporal variation, and the implementation of coarser grids in smooth regions of the flow. Adaption of the rectangular mesh was employed by the overlaying of successively refined layers of grids, with each layer generated from its predecessor by the doubling of the computational cell number in each spatial dimension. Again, further details regarding the algorithm can be found in Falle and Giddings (1993).

4. Results and Discussion

Figure 2 provides an example of a sample stage of solution during the calculation of experiment number 10, using the Reynolds-stress approach to the turbulence closure. From an assembly of a time-lapse sequence of the reaction progress variable such as this, the behaviour of the flame front can be seen to be in-line with expectation. Initially progressing at a relatively slow rate, the reaction zone subsequently accelerates through the unreacted fluid upon each obstacle interaction, returning to a constant velocity in between these areas of turbulence generation.

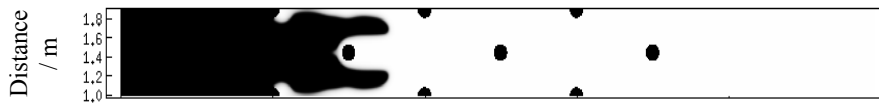


Figure 2. Sample two-dimensional symmetry progress variable predictions of experiment 10.

Analysis of the results provides the maximum overpressures achieved and the flame-front vessel-exit velocities predicted by the models, which are presented in Fig. 3. It is

evident from these results that, in general, the magnitude of the predictions, and hence ultimately their conformity with experiment, depends upon the turbulence model, which in turn has a performance dependency upon the domain geometry and the fuel investigated. This is less evident for the three-dimensional approach, although results based on the Re-stress model are generally more in line with available data.

For the two-dimensional symmetry simulations run involving internal pipe-work, the more reliable Reynolds-stress model is seen to be at variance with its two-equation counterpart with respect to recorded maximum overpressures. Predicted exit flame-speeds do, however, show little difference in the performance of the two turbulence models. At the higher turbulence levels associated with the congested cases, the flow becomes increasingly less isotropic and it appears a notable component of the turbulence stress-tensor is not being represented in the k- ϵ case. Scrutiny of the calculated results also reveals a relative deterioration of the k- ϵ model's predictive ability in the cases of higher hydrogen content, this being due in part to the introduction of hydrogen effecting an increase in both the laminar and turbulent burning velocity, and hence an increase in the turbulence generated. The varied performance of the models is further highlighted when the results obtained from the calculations of the empty rig are considered. Here, conversely to that seen in the relatively high turbulence case, the Reynolds-stress model is seen to predict lower maximum overpressures than its k- ϵ counterpart, over the three fuels considered. Again, predictions of exit flame-speed velocity are similar for the three cases investigated, with little difference observed between the two turbulence model predictions.

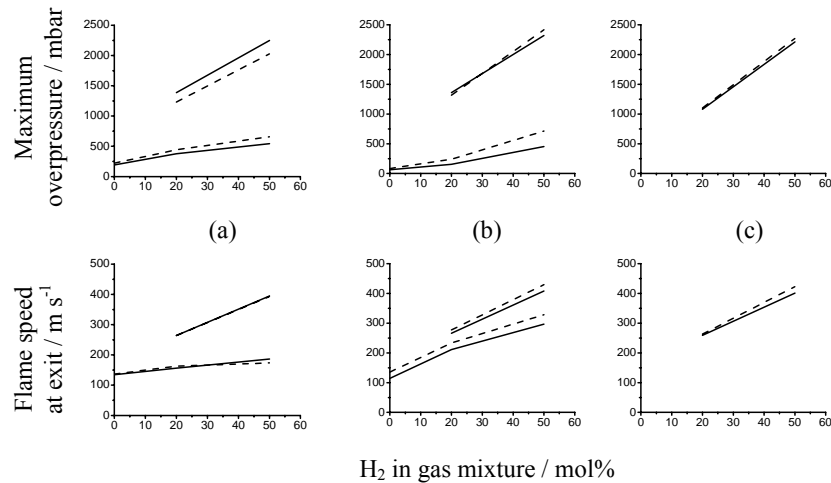


Figure 3. Maximum overpressures and exit flame-speeds obtained using the k- ϵ (dashed line) and Reynolds-stress (solid line) models for the 17-pipe (upper) and 0-pipe (lower) configurations using the (a) symmetry, (b) two-dimensional and (c) three-dimensional approaches.

With reference to the two-dimensional calculations (Fig. 3b), the increase in geometry complexity is seen to bring predicted overpressures more in line in the congested cases, although a less conforming result is seen for the empty vessel. Also, predicted exit flame speeds comply with this observation, which raises questions regarding the validity of the model in such low turbulence regimes. Based on these observations, and the long computational time of approximately 80 hours using a 3 GHz processor, three-

dimensional calculations were undertaken of the high-turbulence cases only, and results are depicted in Fig. 3(c). Both predicted overpressure and flame speed are noted to be of lower magnitude than the previous approaches, with the k- ϵ model typically over predicting Re-stress results in the cases with the higher hydrogen concentration and hence the higher level of turbulence.

One further consideration is the accuracy to which either of these turbulence models can be expected to predict a flow that is substantially laminar, as in the case of explosions within vessels without internal obstacles. Further work has therefore focussed on those experimental tests performed using internal, turbulence generating pipes. Additional investigations are also being undertaken to assess the model's performance in the modelling of similar, but unconfined cases.

5. Conclusions

For the first time, a Reynolds-stress turbulence model has been applied to the prediction of large-scale vented explosions, coupled to a turbulent premixed combustion model. Maximum predicted overpressures and flame-front velocities for five test cases are presented, and comparisons made to calculations based on the k- ϵ model. The Reynolds-stress model is seen to generally be at variance with the isotropic approach, although in terms of predicted overpressures and flame-front velocities these differences are often small. However, the increase in turbulence anisotropy caused by internal pipe work within a vessel necessitates the use of a Reynolds-stress model on physical grounds alone. These observations are valid for the three approaches used to represent the geometry considered, with the level of conformity observed in the two-dimensional cases making them viable for use in future studies.

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