Flash Fire and Burn-Back Hazards in Process Safety Assessment – Some Benefits of CFD Modelling

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The present study examines the feasibility of using both Large Eddy Simulation (LES) and Reynolds-Averaged (RANS) CFD approaches to modelling of transient flash fire burn-back to the source followed by a diffusion controlled jet fire. This study investigates the process in two stages using a simple test configuration consisting of a methane gas jet released vertically into initially still air with a controlled point ignition source downstream. The test configuration is modelled using the CFD packages FDS (Fire Dynamic Simulator) and FLACS, both of which are widely used in oil and gas and process safety assessments. FDS and FLACS feature different turbulent models: LES for FDS and $k-\epsilon$ RANS for FLACS. The first stage of the study involves using both FLACS and FDS to model the gas dispersion from the source prior to ignition and compares the results from each. The second stage involves initiating a controlled ignition downstream of the source and modelling the transient flash-fire burn-back and the subsequent establishment of a jet fire. The flame burn-back to the source is modelled using the FLACS premixed combustion model, the growth of the jet fire from the source is modelled using the FDS diffusion controlled combustion model. This combined approach utilises the strengths of the different CFD solvers for the pre-mixed and diffusive growth regimes to give a more complete description of the evolution from flash fire to jet fire. We conclude that this hybrid CFD approach is feasible, but that further validation against experimental data is desirable.

Keywords: flash fire, CFD, dispersion, jet fire

Introduction

Flash fire hazards are well recognised in the oil and gas and chemical process industries. While the flash fire in itself is generally considered to have rather limited effects, it is recognised that such an event may escalate, into: 1) explosion; 2) fireball; 3) jet fire; 4) pool fire. The first two of these escalated events will require particular geometries of the cloud and/or its surroundings to be present, but do not require complete burn-back to the source. The latter two require burn-back, but are potentially also affected by the release source, the presence of obstacles, terrain effects and prevailing atmospheric conditions. Inclusion of such complex effects usually requires Computational Fluid Dynamic (CFD) modelling.

An example of a flash fire incident which resulted in serious consequences occurred in 2007, when a propane leak ignited at the Valero McKee Refinery in Sunray, Texas, US. Three workers suffered serious burns, and the refinery was forced to shut down. The fire began following a leak in the propane deasphalting unit. The wind blew the vapour cloud towards a boiler house, where ignition occurred and flames burned back to the cracked pipe that leads to the formation of a high pressure jet fire, which soon escalated to more fires over a greater area, according to a study from *U.S. Chemical Safety Board (CSB), 2007* [1].

In most safety and risk assessment study, the flash fire is modelled rather simplistically, e.g. by assuming that the fire covers the dispersion footprint, LFL or ½ LFL. However, the transient nature of flame propagation and the often non-homogeneous gas cloud make it a more complicated phenomenon. During vapour cloud formation, depending on the velocity of the fuel-air mixing process, the composition of the bulk of the fuel vapour cloud will be ultra-lean (i.e., below the lower fuel-air flammability limit) in the case of fast mixing, ultra-rich (i.e., above the upper flammability limit) in the case of slow mixing (Fig.1), or flammable (i.e., within the flammability limits) in the intermediate case (Fig.2), according to *Hu, 2008* [2]. The fast mixing case corresponds to a desirable safe dispersion scenario in which there is no fire or explosion hazards, while the latter two can develop into significant fire and explosion events following successful ignition. In the case of an ultra-rich fuel vapour cloud, combustion corresponds predominantly to a diffusion burning mode (Fig.1c); in the case of a flammable fuel vapour cloud, combustion includes an intense premixed burning mode (Fig. 2c), which is usually termed as flash fire.

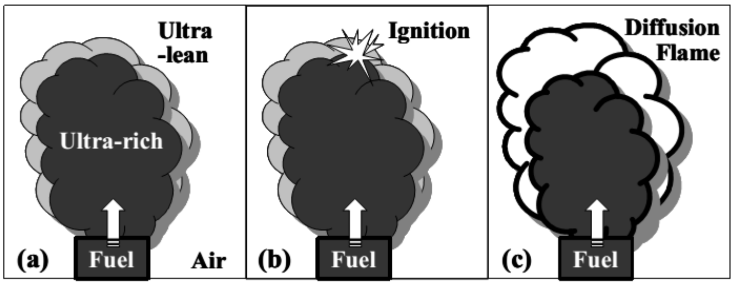

Figure 1: Problem configuration corresponding to (a) the formation of a large ultra-rich fuel vapor cloud, followed by (b) ignition and (c) diffusion burning

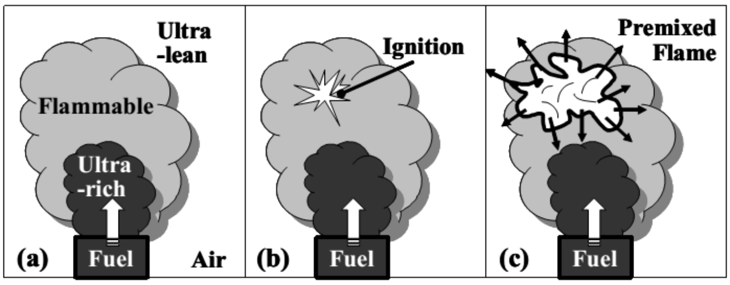

Figure 2: Problem configuration corresponding to (a) the formation of a large flammable fuel vapour cloud, followed by (b) ignition and (c) deflagration

Despite considerable understanding of flash fire from *Rew etc., 1996* [2], many of its details have often been neglected in process safety. CFD provides a means to bridge the gap between theory and risk assessment in practice. In this study we shall investigate the gas dispersion, flash fire burn-back and subsequent establishment of a jet fire using CFD for a simple scenario of a vertical buoyant gas (methane) released into still air and ignited downstream. The rationale behind choosing a simple scenario is that it lends itself to comparing results for the simplest non-trivial case and allows comparison with simple correlations. Also, it easy to imagine that this configuration might also be modelled within the laboratory as a means of validating the CFD models. Unfortunately we do not have the means to conduct such a laboratory study, but we can do a numerical 'experiment' using CFD. A two-stage modelling process is adopted here. The first stage looks at the non-homogeneous dispersing cloud from a continuous source, using two numerical tools FLACS [4] and FDS [5] (Fire Dynamic Simulator). Each CFD solver features a different turbulent model: $k - \epsilon$ RANS (Reynolds-Average Navier-Stokes) model for FLACS and LES (Large Eddy Simulation) model for FDS. A comparison between the gas dispersion predicted using these two different approached is conducted. The second stage combines the advantages of both CFD solvers, premixed combustion for FLACS and diffusion controlled combustion for FDS. A controlled ignition is initiated in the downstream of dispersion field established, the premixed combustion event is modelled using FLACS up to the point where the flame front has reached to the boundary of flammable gas range, then the phenomena can be treated as switching to a gas jet fire, which is a diffusion combustion event that is capable to be modelled by FDS.

Numerical Set-up

An idealised configuration of methane gas released vertically into initially still air is used for this study, ignition is initiated when a steady state dispersion field has been established. As illustrated in Fig.3, the computational domain is a rectangular box of 8.2 m x 8.2 m x 20 m in x, y, z direction, with boundaries open to all sides. An upward directed methane gas source is placed at 3 m height from floor in the middle of the box. The source is square of dimension 0.5 m x 0.5 m with methane gas released at a steady flow rate of 5 kg/s uniformly over this area. An ambient temperature of 20 °C is specified for both the source and air, which corresponds to a methane density of 0.66 kg/m^3. The source velocity is 30 m/s. The resulting release is hence an upward buoyant sub-sonic jet. The geometry has deliberately been kept simple in order to highlight different behaviours for the CFD modelling of gas dispersion, premixed combustion and diffusive combustion when the main turbulent source is the jet itself. In particular, the source is sub-sonic allowing both FLACS and FDS to model dispersion directly from the source location without having to resort to sonic-expansion models.

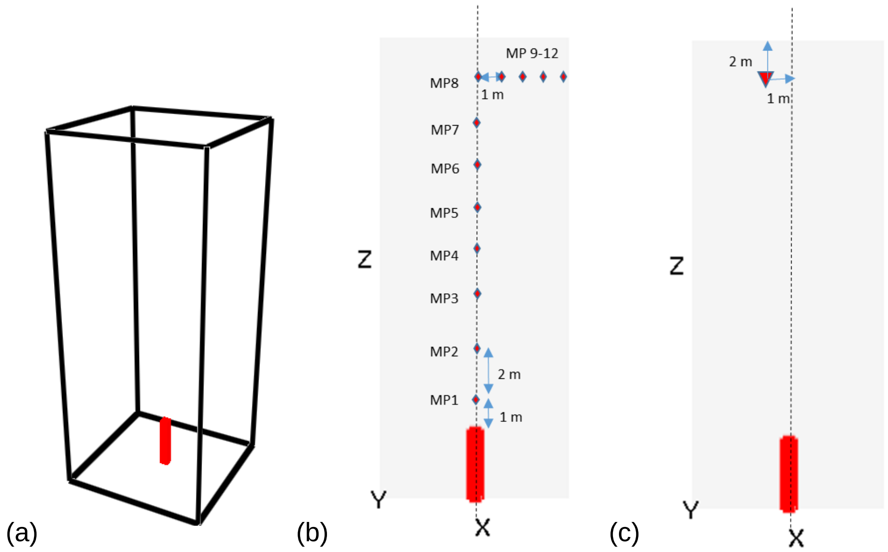

Figure 3: Numerical experiment with methane dispersed upwards: (a) 3D configuration, release from top of the red box; (b) Monitor points location in a domain central plane for dispersion verification study in Section 3, monitor point denoted by red diamonds; (c) Ignition location in a domain central plane for fire initiation, at 8s upon start of release in combustion case, location denoted by red triangle

A uniform grid of 0.1 m is used for both the gas dispersion modelling and the fire modelling. This meets the modelling guidelines of both FLACS and FDS. Turbulence in FLACS is accounted by $k - \epsilon$ model at subgrid level (<Δ=0.1m), while in FDS a variation of

Deardorff's model is used to close the turbulent viscosity term, $\mu_t = \rho C_v \Delta \sqrt{k_{sgs}}$, with a LES filter width Δ=0.1m. Since the reaction zone in a premixed flame is thin compared to practical grid resolution, the combustion model in FLACS uses a factor β to increase diffusion and thicken flame zone and meet the requirement that the grid size should be smaller than flame thickness. The minimum flame thickness in the FLACS model is currently set at approximately 3 grid cells [4]. In FDS, a grid size δ_x is usually required to solve the buoyant plume flow field with a non-dimensional expression D^*/δ_x, where D^* is a characteristic fire diameter, $D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}}\right)^{2/5}$, and $\dot{Q}$ is the total heat release rate of the fire.

While in FDS the boundary of the computational domain is set as 'OPEN', in FLACS the boundary of the computational domain is chosen to the 'NOZZLE' type, which is similar to EULER type boundary but more robust, and is the default outlet boundary condition for dispersion simulations.

Gas Dispersion

The numerical experiment is firstly performed only with gas dispersion, i.e. no ignition is energised. The dispersion field predicted by FLACS and FDS are illustrated in Fig.4 and Fig. 5, at 2 s, 5 s and 10 s from the start of release. Both simulations give similar shape of plume as plume develops, although some differences at the open boundary are noticed In the FLACS simulation the gas flow out of the domain appears to be limited such that plume becomes artificially wider near the top of the domain.

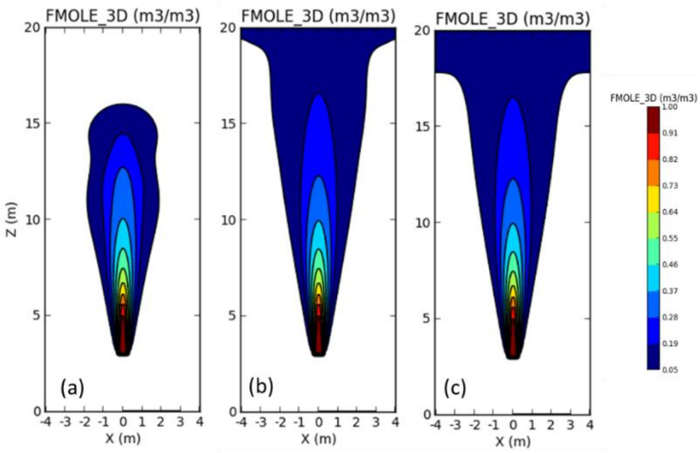

Figure 4: Methane dispersion field modelled by FLACS at (a): 2 seconds; (b): 5 seconds; (c): 10 seconds, from start of release. The outer boundary of the plume denotes the LFL level, which is 5% by volume in air.

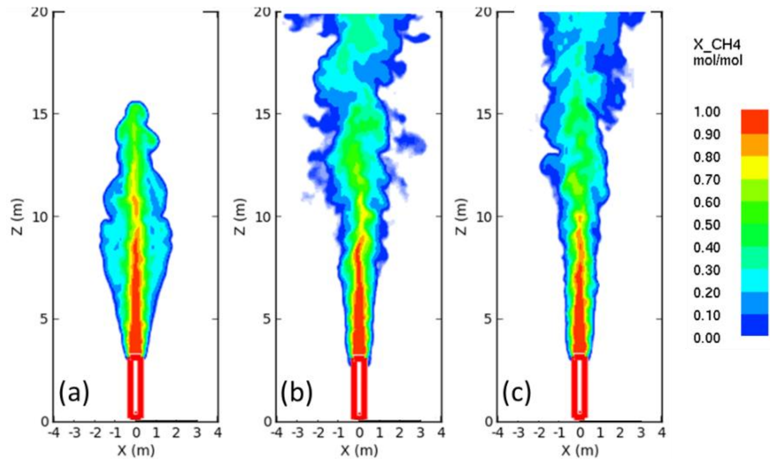

Figure 5: Methane dispersion field modelled by FDS at (a): 2 seconds; (b): 5 seconds; (c): 10 seconds, from start of release. The outer boundary of the plume denotes the LFL level, which is 5% by volume in air.

To further investigate the top boundary issue in the FLACS simulation, two more simulations are performed: 1) enlarged domain from 8.2 m x 8.2 m x 20 m in x, y, z direction to 12.2 m x 12.2 m x 30 m in x, y, z direction; 2) refined grid size of 0.05 m. In both cases the release location and size remain unchanged. The comparison between these two additional cases and the original FLACS simulation is shown in Fig.6. Moving the boundary further away (Fig. 6b) reduces the widening of the jet, confirming this to be a boundary effect. Using smaller grid spacing (Fig. 6c) results in a slight increase in the predicted distances to the plotted contour levels, however, such differences are probably not very significant within the context of risk assessment

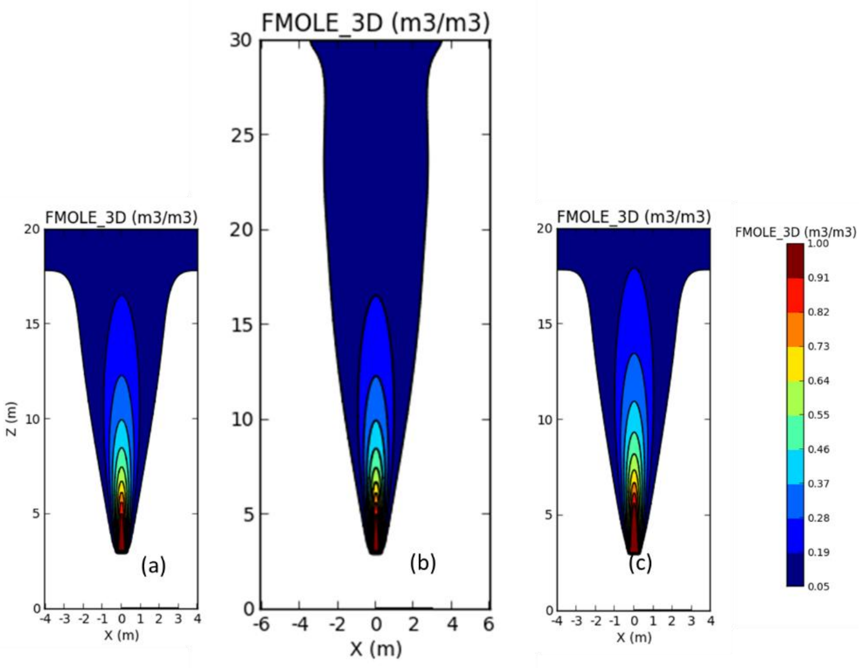

Figure 6: Methane dispersion field modelled by FLACS at 10 seconds from start of release (a): original domain, 0.1 m grid; (b): enlarged domain, 12.2m x 12.2m x 30m, 0.1 m grid; (c): original domain, 0.05m grid. The outer boundary of the plume denotes the LFL level, which is 5% by volume in air.

Time-Averaged Concentration Profiles

The CFD dispersion results indicate that between 5 and 10 seconds after release, the plume can be considered to have reached an approximate steady state. It is instructive to compare the steady-state time-averaged concentrations from the FLACS and FDS simulations with each other and with empirical correlations.

Figure 7 shows the variation of time-averaged fuel concentration predicted along the jet centreline for both FDS and FLACS. The time-averaging is applied to the results between 5 and 10 seconds only. Also shown is the predicted centreline concentration variation using an empirical jet correlation due to Chen & Rodi (see Appendix A of this paper for how the correlation is modified to account for a non-ambient density source and divergence avoid close to the source). The empirical correlation provides a useful validation check since it gives an indication of the centreline concentration behaviour observed for real sub-sonic jets. The mean concentration predictions for all the measured centreline points lie above the Upper Flammable Limit (UFL) of methane which is approximately 15% vol/vol.

The FLACS predictions for the 0.1m and 0.05m grid spacing are similar to each other, confirming the observation from the contour plots that the predicted concentration field is not significantly changed by the grid refinement. Compared with the FDS predictions and the modified Chen & Rodi correlation, the FLACS results show a more rapid decay in concentration with distance close to the source. This difference close to the source might reflect differences between the source turbulence in the models and consequential differences in predictions of the flow development region of the jet – FLACS is initialised according to guidance with a turbulence intensity and turbulent length scale based upon the initial source size, whereas the turbulence in FDS develops subsequent to the source, which would cause a difference in turbulent eddy diffusion. The FLACS, FDS and modified Chen & Rodi correlation predictions are in closer agreement further downstream. Generally the modified Chen & Rodi correlation gives values between the FDS and FLACS predictions, but closer agreement with the FDS predictions at greater distances.

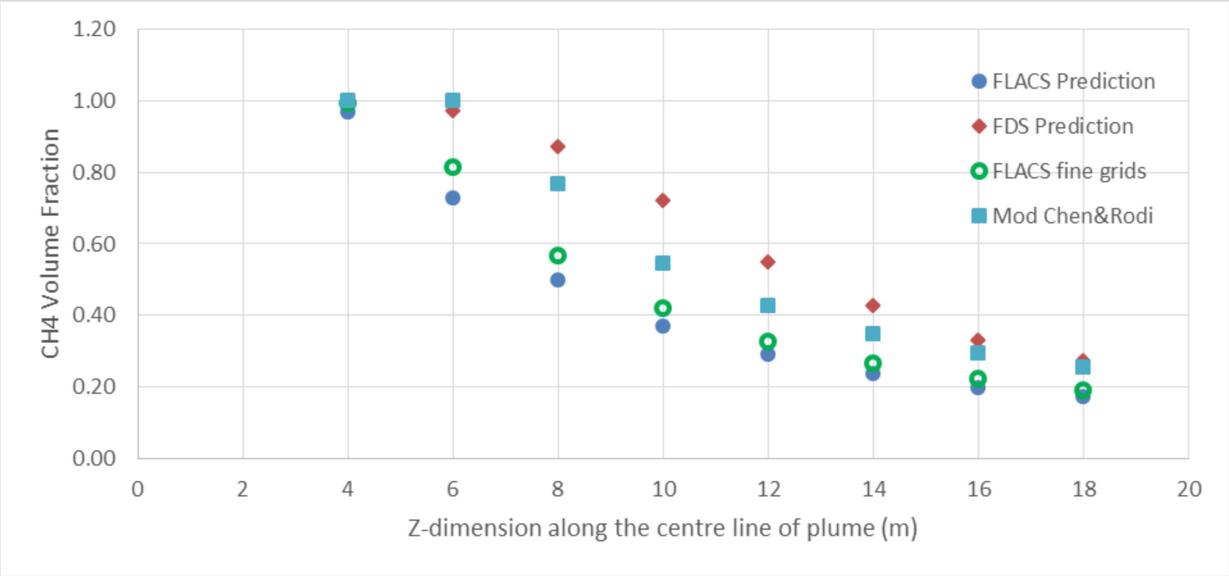

Figure 7: Methane concentrations predicted by FDS and FLACS at centreline monitor points (MP1-MP8 as illustrated in Fig.3b), results are time-averaged between 5 and 10 seconds upon start of release. 1) Blue circle – FLACS prediction as in Fig.4; 2) Red diamond – FDS prediction as in Fig.5; 3) Green circle – FLACS prediction as in Fig.6c; 4) Blue square – modified Chen & Rodi correlation as in Eq.8 in Appendix A

Figure 8 shows a comparison of the lateral mean concentration profile by FDS and FLACS at a height of 18m. Again the concentrations are time-averaged of the predictions between 5 and 10 seconds. The higher centreline prediction of FDS at this height is evident with a concentration of approximately 28% vol/vol for FDS compared with 17% vol/vol for FLACS. Plume widths, as determined from the lateral distance to ½ centreline concentration are approximately 1.7 m for FLACS and 1.3 m for FDS. Both FLACS and FDS predict that the mean concentration field falls below UFL at similar lateral distances from the centreline - approximately 0.8 m for FLACS and 1.2 m for FDS. The flat concentration tail for FLACS which is not present in the FLACS large domain confirms this to be a boundary induced artefact.

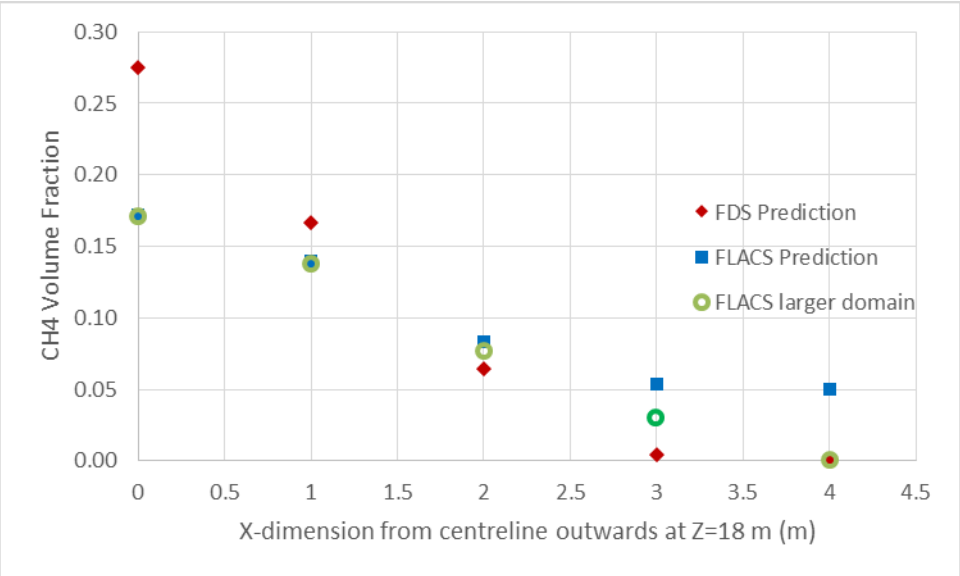

Figure 8: Methane concentration predicted in different case at monitor points across the plume at Z=18m (MP8-MP12 as illustrated in Fig 3b). 1) Blue square – FLACS prediction as in Fig.4; 2) Red diamond – FDS prediction as in Fig.5; 3) Green circle – FLACS prediction as in Fig.6b

Flash Fire Burn-Back

The second stage of the study involves introducing a controlled ignition and modelling the flash fire burn-back to the source and the subsequent development of a jet fire. The flash fire burn-back is modelled using FLACS premixed combustion model starting from the steady state gas concentration field predicted by FLACS $k-\epsilon$ RANS dispersion model.

Modelling is undertaken for an ignition source placed at the ignition location illustrated in Fig 3c. This ignition location lies close to the UFL boundary of the mean concentration filed. Fig.9 illustrate the burn-back of the flame as predicted by FLACS from 0.1 s up to 2 s after the time of ignition. The flame front appears smooth in the beginning, and the flame propagation is entirely governed by thermal and/or molecular diffusion process. Shortly after, the flame surface becomes wrinkled due to a few factors such as flow dynamics and concentration effects on flame speed, e.g., at the flammable limits, particularly LFL, the flame speed is significantly lower than its maximum when the mixture is close to stoichiometry. After a transition period, the flame eventually reaches the turbulent burning regime, which features a much faster flame propagation speed than the initial laminar speed [4]. For the case being modelled, the flash fire flame reaches the release source in less than 1 second.

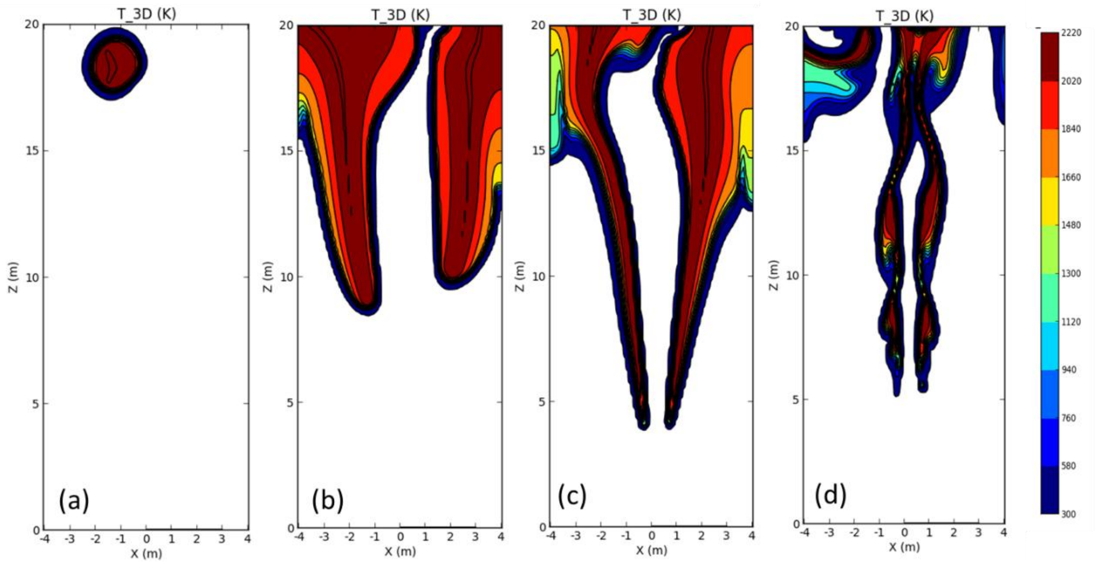

Figure 9: Temperature field illustrates the flash fire propagating through the flammable mixture at different times after ignition. (a) 0.1 second; (b) 0.5 second; (c) 1 second; (d) 2 seconds.

We have modelled the flash fire stage using only FLACS because FDS lacks the premixed combustion capabilities which are present in FLACS. Unfortunately this means that we are unable to investigate burn-back in the more 'dynamic' concentration field characteristic of an LES model such as FDS.

Jet Fire

When the flame propagates back to the source as shown in Section 0, there is a possibility that the source of release would be ignited and a turbulent diffusion jet fire would develop. Modelling of the turbulent jet fire growth has been undertaken here using the FDS diffusive combustion model. Fig.10 shows the predicted jet fire temperature field at 2 s, 5 s and 10 s after ignition of the source gas (these times are measured from the point at which the flash-back reaches the source). In contrast to the flash fire that propagates from the remote ignition source to the release source in less than 1 second, the diffusion jet fire propagates is much slower, not surprisingly developing over a similar time-scale to the initial gas dispersion as illustrated in Fig. 5.

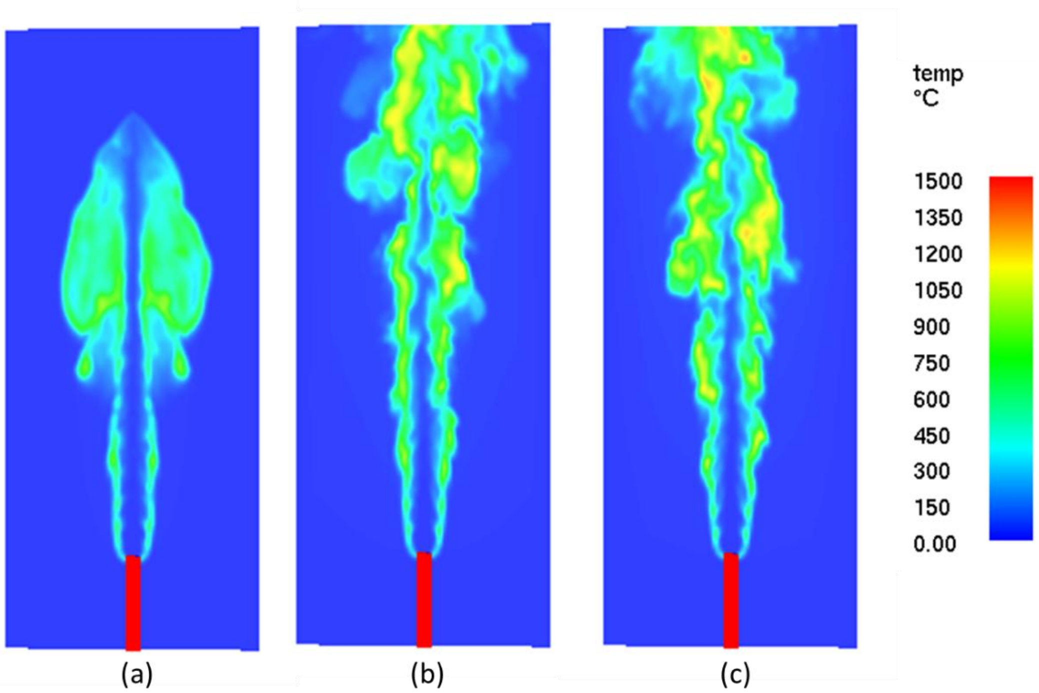

Figure 10: Temperature field illustrates the jet fire originating from the release source upon its start on the flash-back at different time: (a) 2 seconds; (b) 5 seconds; (c) 10 seconds.

Discussion

In this study we have used both LES and RANS CFD approaches to investigate the gas dispersion, flash fire burn-back to the source and subsequent jet fire for the idealised configuration of a methane gas jet issuing into initially still air. The advantage of this idealised configuration is that mixing is dominated by jet turbulence and the geometry is sufficiently simple to allow comparison with empirical jet correlations and to see differences between different CFD approaches in the absence of other complicating factors such as obstacles. Two commonly adopted CFD models have been used: namely FDS (using an LES approach) and FLACS (using a $k - \epsilon$ RANS approach).

We have modelled gas dispersion using both FDS and FLACS and compared their predicted concentration fields, including a comparison with empirical correlation for centreline time-averaged concentration. For the modelled case, FDS predicted higher time-averaged concentrations, especially close to the source, but these differences diminished with distance and overall the time-averaged dispersion results are rather similar. Greater differences between model predictions might be expected for more complex situations.

As expected the LES model (FDS) shows a more dynamic concentration field compared the RANS model (FLACS) which implicitly averages over the turbulent fluctuations. This might have implications for burn-back to the source, for example turbulent fluctuations in the concentration field from an LES model may not always support burn-back to the source even if based on averaged fields it does.

An important aspect for CFD models is whether their combustion sub-models are suited to pre-mixed or diffusion controlled combustion. We have used the FLACS pre-mixed combustion model to model flash fire burn-back to the source, whereas we have used FDS diffusion controlled combustion model to model development of the jet fire. This hybrid approach combines recognised strengths of both CFD solvers. Our study shows that it is feasible to use FDS and FLACS in this way. A similar combination of combustion sub-models is now offered by GexCon (the developers of FLACS) in the FLACS Fire extension to FLACS.

Real accidental release scenarios will, of course, be more complicated than what is modelled here, especially if there are sufficient obstructions in the flammable cloud, the flame may accelerate such that significant overpressures are produced, giving an unconfined vapour cloud explosion. In windy condition, the wind/flame interaction could also cause the flame propagation process to speed up, slow down or cease, depending on a number of factors such as the wind conditions and dispersed cloud characteristics. Ultimately, burn-back to the source is dependent upon cloud inhomogeneities, including intermittency and connectivity between different flammable gas pockets. A jet with high strain rate would also contribute to flame extinction. By their nature these complex aspects are difficult to model and validate and perhaps CFD is currently the only viable approach to account for these. Improved confidence in applying CFD to such complex situations follows from an understanding of the behaviour of CFD models for simpler scenarios, and building up including more effects in a 'stepwise' manner. In our view, a reasonable next step from our study would be validation against experimental measurements for a similar configuration including dispersion, ignition, flash fire burn-back and establishment of a jet fire. It is quite possible that such experimental data already exists, but we are currently unaware that FLACS and FDS have been validated against these.

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Appendix A – Empirical Correlation for Mean Centreline Concentration

Following study on turbulent jets and plumes by *Rodi, 1982* [6], we present empirical expressions for the centreline decay of a gas jet, based on dimensional arguments involving the following conserved fluxes: 1). Contaminant mass flux, *Y* 2). Momentum flux, *M.*

It should be noted that conservation of momentum, *M* is dependent upon there being no ambient flow and buoyancy induced velocity being negligible. Hence conservation of *M* is reasonable for a jet in still air whilst velocity is large, but eventually for a non-ambient density release gravitational buoyancy forces will change *M*.

Assuming uniform profiles at the orifice (with orifice quantities denoted by subscript 0)

$$Y = \rho_0 A_0 u_0 \quad (1)$$

and

$$M = \rho_0 A_0 u_0^2 \quad (2)$$

where

ρ_0 is the density of the released fluid

A_0 is the area of the orifice

u_0 is the velocity at the orifice

At a sufficiently large distance *x* from the orifice, only the conserved quantities are 'remembered' and on dimensional grounds [6], it is argued that the concentration should only depend on distance *x* together with *Y*, *M* and the ambient fluid density, ρ_a. This leads to the centreline concentration on a mass per unit volume basis, $C_{m/v}$ being given by

$$C_{m/v} = \frac{\rho_a^{1/2} a\, Y}{M^{1/2} x} \quad (3)$$

where a is an empirically determined constant. According to [6] Chen and Rodi (1980) give a value of $a = 5.64$ for circular axi-symmetric jets, whereas Birch et al (1978) give a value closer to 5.8 in the region beyond 30 exit diameters.

We note that the above expression differs slightly from that given in [6] due to inclusion here of density in the definition of momentum flux, leading to the requirement for including the $\rho_a^{1/2}$ term in the numerator on dimensional grounds.

The concentration on a volume per unit volume basis, $C_{v/v}$ is then given by

$$C_{v/v} = C_{m/v}/\rho_0 \quad (4)$$

and on a mass per mass basis $C_{m/m}$ is approximately

$$C_{m/m} = C_{m/v}\rho_a \quad (5)$$

which is only strictly true when the density of the mixture is close to that of the ambient fluid.

For a circular source

$$A_0 = \frac{\pi}{4} d^2 \quad (6)$$

which results in

$$C_{m/v} = K(\rho_0\rho_a)^{1/2}\frac{d}{x} \quad (7)$$

$$C_{v/v} = K\left(\frac{\rho_a}{\rho_0}\right)^{1/2}\frac{d}{x} \quad (8)$$

$$C_{m/m} = K\left(\frac{\rho_0}{\rho_a}\right)^{1/2}\frac{d}{x} \quad (9)$$

where $K = \frac{a\pi^{1/2}}{2} = 5$ based on the Chen and Rodi (1980) value for a.

The above empirical expressions are not expected to be valid close to orifice. In fact the 1/x dependence implies concentrations greater than pure and infinite at x=0. A practical way of avoiding this divergence is to cap the concentration prediction by that at the source, but it should be noted that at best this is only a crude approximation for this region.