

## ADVANCES IN HAZARD ANALYSIS USING CFD

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Computational Fluid Dynamics predictions of several types of industrial hazards are presented. The capabilities of the CFD models are assessed for the following applications: explosion in linked vessels; fire on an offshore platform; semi-confined fires; oil pool fire; oil dispersion and burning at sea; and ammonia dispersion from a barge in a canal. The calculations compare favourably with available experimental results. Developments in parallel processing which improve the efficiency of the simulations are also presented in this paper.

Keywords: CFD, explosion, fire, pool-fire, oil-leakage, gas-dispersion

### 1. INTRODUCTION

Industrial hazards can derive from many different circumstances, leading to potentially devastating accidents, including liquid spillages, gas leakages, fires and explosions. Understanding the physical processes which occur during such accidents can be useful in several ways. At the design stage, plant, equipment and buildings can be designed for survivability and to limit the impact of an accident should one occur. For existing facilities, a more complete understanding of accident scenarios can help in formulating effective emergency procedures.

Since full-size experimental tests can be extremely costly or impractical to perform, and because small-scale tests may not scale up accurately, a viable alternative is required. Computational fluid dynamics (CFD) techniques offer an effective means of simulating the complex physical flow phenomena encountered in many accidents. Because of the increased use of CFD software for safety analysis, the field is maturing rapidly and considerable progress is being achieved in validation and understanding, which in turn leads to the development of better models.

The main objective of the present work is to demonstrate the potential of general-purpose CFD software for hazard analysis by quoting from previous applications. Specific cases which illustrate this are described here:

- explosion in linked vessels
- semi-confined fires
- fire on an offshore platform

- oil pool fire
- oil dispersion and burning at sea
- ammonia dispersion from a barge in a canal

Some results given here are new, specifically in relation to semi-confined fires.

Finally, some developments in computer hardware are discussed, which should lead to significant improvements in the ability to predict industrial safety problems reliably.

## 2. MATHEMATICAL MODEL

The present contribution illustrates previous use of AEA Technology's general purpose CFD software, CFX 4, to perform the calculation. This solves the full Navier-Stokes equations which describe fluid motion. The mathematical model and the solution procedure are well known and will not be repeated in detail here [1].

The features of the software which are of particular importance in the simulation of safety-related applications include advanced physical models for turbulent, combusting and multiphase flows, the use of 'unstructured multi-block' meshes which can efficiently simulate the most complex of geometries, and higher-order numerical differencing schemes which ensure accuracy of the solution.

## 3. CFD SAFETY-RELATED APPLICATIONS

### 3.1 Explosions in Linked Vessels

A number of simulations of explosions and deflagrations in confined, or partially-confined, spaces have been performed. In the solution procedure, the three stages of the deflagration are simulated: firstly the ignition phase; then a laminar and low-turbulence thin-flame phase, and finally a high-turbulence thick-flame stage. The software also accounts for suppression of combustion through quenching due to excessive flame stretching.

An example of this type of application involves the simulation of an explosion in linked vessels for which experimental results are available [2]. The apparatus consists of two cylinders of 0.5m diameter and 0.5m length connected at their axis by a 1.7m-long pipe of 76mm diameter. The apparatus is initially filled with a ten per cent methane/air mixture and is ignited either at a point in the centre of the vessel or at the closed end.

For both types of ignition, the flame grows slowly until it reaches the connecting pipe, when it accelerates while travelling the length of the pipe. When the flame exits the pipe into the second vessel, flame speeds increases dramatically causing a violent explosion. The numerical calculations predict well the explosion [3] as shown in Figures 1 and 2 which compare the calculated and measured overpressure histories for the central ignition case for both vessels.

The overpressure distribution in the vessel can be integrated numerically to provide total loadings on the structure. Further calculations have been performed and validated against data on baffled enclosures [4]. With such models, the CFD procedure can be used with confidence to predict many potential explosion scenarios, and to determine the survivability of the structure.

### 3.2 Semi-Confined Fires

CFD is frequently used to simulate the development of fires in buildings and to determine the movement of smoke [5,6]. The resulting understanding of how a fire progresses can allow designers to optimise the positions of sprinkler, ventilation and fire-fighting systems and to plan emergency procedures.

A CFD study to investigate the effects of external ventilation on a fire in a building has been commissioned by the Home Office. The aim of the project is to deliver guidelines to the fire services in the matter of tactical ventilation. This involves creating openings to allow fire-fighters to enter buildings and attack the fire sources, even if these feed the fire with fresh oxygen.

The CFD has been validated against experiments consisting of heptane pool fires (nominal power of 11MW) in an industrial building. These experiments have been undertaken by the Home Office's Fire Experimental Unit (FEU) at the Fire Service College, Moreton-in-the-Marsh, England.

The building which is about 17m long and 9m wide, contains two floors, a basement, doors, and windows. Its roof is pitched unsymmetrically, with a mean height of about 5m and includes a number of roof vents (see Figure 3). The experiments involve igniting the fire in the closed room condition, and opening various combinations of doors and vents after five minutes.

As the fire can be starved of oxygen, the fuel burning rate is not constant and the fuel evaporation is dependent on radiative heat transfer. This is taken into account in the simulation by coupling radiation and the fuel evaporation. Combustion is modelled with the eddy break-up model and radiation is calculated using Shah's discrete transfer method available in the chosen software.

Even when the building is nominally sealed, many leakage paths exist around closed doors, windows, vents and especially through many holes penetrating three of the compartment's walls at a low level, just above the floor. These building leakages are modelled as combinations of (a) explicitly-modelled resistances at doors and vents, and (b) sources/sinks of mass where the size of the leakage paths are small relative to the computational cells. As a first stage, all the leakages have been specified at the four explicit apertures, namely two doors and two vents.

The simulation shows that the pressure initially rises inside the compartment, which expels some of the oxygen which would have otherwise fed the fire. When the fire is starved of oxygen, it decays and pressure inside the building drops to less than atmospheric pressure. This allows fresh air to re-ignite the fire, and clearly the fire dynamics depends on the ease with which fresh air can be sucked in and advected to the fire.

The experiments exhibit the classical stratification. CFD computations in a perfectly scaled model of the building, and in a well-ventilated state (with both doors and vents open) also reveal ample stratifications. However, preliminary analysis of the nominally closed state including the leakages led to a collapse of the stratification within a few minutes. The results have since been improved upon substantially, and recent indications are that during the nominally closed phase it is necessary to account for actual

locations and magnitudes of the leakages and wind effects. Inadequacies of the  $k-\epsilon$  turbulence model may also be an issue but at this stage it is considered to be less important than the above.

Typical results are shown in Figure 4, in which the temperatures in a vertical line, at five locations spaced 1.0 metre apart above the floor, are shown as functions of time during the closed phase. Ongoing calculations are evaluating the field after opening of various doors and vents. These are preliminary results and additional information will be published at a later date.

### 3.3 Fire on an Offshore Platform

CFD has proved particularly valuable in the analysis of fires on offshore platforms, and in assessing the viability of escape routes. The presented CFD procedure can calculate the external pressure levels around temporary safe refuges and determine the extent of smoke ingress and therefore the integrity of the refuge.

Figure F1 shows the results of an analysis of wind effects on a fire due to a gas leak on an offshore oil and gas platform [7]. The rate of gas leakage is 7.5kg/s, whilst the platform is subject to a southerly wind of 30m/s. Temperature contour plots are used to track the path of the resulting hot plume, and smoke concentrations are calculated at points of interest.

This type of study allows quantitative assessment of the conditions to which rig personnel and equipment would be exposed in the event of an accident. Parametric studies can easily be performed, providing a comprehensive understanding of safety matters under all conditions, such as varying wind speed and direction.

### 3.4 Pool Fires

CFD simulations can be used to predict the propagation of liquid spillages, which can occur during the handling of fuels such as oil or petrol. Furthermore, CFD can predict the effect of spillage fire should this occur and calculate the radiative heating of remote structures.

Recently, pool-fire tests have been used to validate further the combustion models in the present CFD procedure [8]. The results are presented in Figure 6, which displays an overlay of a video-based image of the real fire and the predicted iso-surface of constant temperature slightly above the ambient. The figure shows that the predictions are in good agreement with the experimental results. The experiments also yield an effective flame inclination to the vertical of 40 degrees, which compares well with the value of 37 degrees predicted by the CFD software.

### 3.5 Oil Dispersion and Burning at Sea

A safety issue of concern in relation to the operation of offshore installations involves the jettisoning of oil into the sea in order to reduce the risk of escalation during an accident aboard the platform. A CFD analysis has been carried out to examine the effect of dispersion of the oil within the sea and the behaviour of a fire as a result of the oil slick igniting [9].

The physics of waves, currents, and oil slicks are complex. For the dispersion modelling it has been assumed that the only background motion (where background

refers to the motion prior to the oil being jettisoned) in the sea is that which is driven by wind shear at the sea surface. Thus, the mean sea current flows in the same direction as the mean wind direction.

The complications of wind-wave interactions have been simplified greatly by adopting a plane air-sea interface and imposing a mean shear stress, based on correlations from oceanography. Several sea states have been considered in the study, however, this illustration concentrates on one case where there is a wind of 10m/s (at a height of 10m above the mean sea level).

The oil dispersion problem is, in reality, a multiphase, multi-component phenomenon involving oil, water and air. To simplify matters, the work described here models the mixture as a homogeneous two-phase medium made up of water and dispersed oil and any air which is entrained by the oil or by waves at the sea surface is neglected. The term homogeneous refers to the modelling assumption that there is no slip between the oil and the water. Thus, the behaviour has been modelled by adding a partial differential equation for the oil volume fraction  $\alpha$ , and an equation of state which represents changes in density due to the presence of oil. Variations in  $\alpha$  lead to inhomogeneities in the density and hence to buoyancy forces. These forces drive the oil upwards, and turbulent diffusion drives the oil away from regions of high concentration.

The oil which is jettisoned is represented as a round source at the sea surface. The source of stabilised crude oil at the water surface is active for only a finite period of time during the transient simulation.

The mesh for this calculation was step-shaped in a vertical plane and wedge shaped in a horizontal plane. The step was deeper in the vicinity of the jet entry point to allow for the penetration of the jet in this region. In the horizontal plane, the mesh stretched 1040m in the wind direction (40m of it upwind of the source). The narrowest and widest edges of the wedge were 100m and 612m respectively.

The background state was determined by carrying out a steady-state calculation in the absence of any oil. The predicted flow pattern of the oil is shown in Figure 7, while Figure 8 and 9 depict the slick thickness at two instants. Initially the jet is driven downwards, however, as the oil rises it attempts to spread radially, which it is less able to do in the upwind direction. This results in a build up of oil which spreads cross-wind to generate a slick with the profile shown in Figure 8. This lateral dispersion leads to a bifurcation of the slick as shown in Figure 9.

The likelihood and method of ignition have not been studied. Instead it has been assumed that the slick will burn wherever and whenever its thickness is greater than some critical value.

A separate simulation is set up within the atmospheric layer, with its lower boundaries coinciding with the mean sea level. In the present wind scenario, the mesh is rectangular with the following dimensions:  $-30\text{m} < x < 250\text{m}$ ,  $0 < y < 125\text{m}$ ,  $0 < z < 100\text{m}$ , where  $x$  points downwind,  $y$  crosswind and  $z$  vertically upwards. The origin coincides with the position at which the oil enters the sea.

The results of the dispersion calculations are used to provide boundary conditions relating to the location and extent of the fire region. The oil thickness from the dispersion calculations is modified with time to take account of any burning.

Typical results are presented in Figures 10 and 11. These show a complicated flame shape that can bifurcate even if the source is not bifurcated [9]. Figures show the situation late on, at 180 seconds after the initial oil release. At this stage the fire source is bifurcated and so the side view in Figure 10 has been produced in the vertical plane  $y=29\text{m}$ . Figure 11 depicts the soot temperature contours at a height which corresponds to the ventilation intake to the muster area.

### 3.6 Gas Dispersion from a Barge

For large-scale environmental and pollution studies, experiments may be impractical or impossible to perform, in which case CFD is the only available approach, especially in the study of gas-leak dispersion, and the build up of toxic or flammable gases [10].

In a recent environmental study, CFD has been used to simulate the leakage and dispersion of gaseous ammonia from a barge in a canal. The ammonia leaks at a rate of 0.05 kg/s and is entrained by the wind, though some tends to stagnate in the low pressure region behind the barge. Several wind directions have been analysed. Figure 12 and 13 show the position of ammonia cloud for different wind configurations.

CFD simulations of gas dispersion problems offer more flexibility than, for example, the standard Gaussian methods as they permit complex topology and atmospheric conditions to be considered easily. Parametric studies of gas dispersion rate, water level in the canal, wind direction and speed can be performed to provide a complete understanding of the possible accident scenarios.

## 4. FUTURE DEVELOPMENTS

One of the limiting factors in the use of CFD software is the large computation time which highly dynamic problems can require. Low cost parallel processing systems are now becoming available, built around standard workstation technology. The European Community project, CFX/D is aimed at disseminating the benefits of high performance computers in fire and safety simulation. Early results from the project are showing typical speed-ups on practical industrial problems by a factor of 3 or more on four processors. With bigger problems, the speed-up can be greater still. Increased performance of this magnitude will facilitate the use of finer computational meshes, more complex physical models, and more exhaustive parametric investigations to be performed.

## 5. CONCLUDING REMARKS

The cases presented in this paper demonstrate the increased maturity of CFD for the simulation of many safety-related fluid flow and heat transfer phenomena. This has led to its application by engineers and scientists to many more safety related applications and it is now a useful additional tool for the assessment of major hazards.

## 6. ACKNOWLEDGEMENTS

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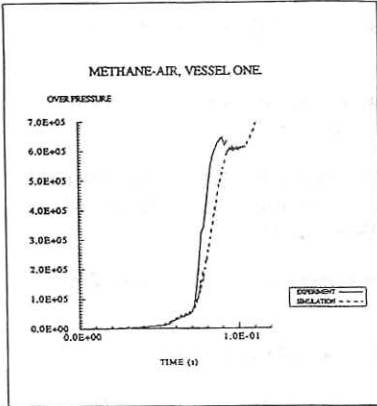


Fig. 1: Explosion in linked vessels - comparison between experiment and simulation for the pressure history in the first vessel.

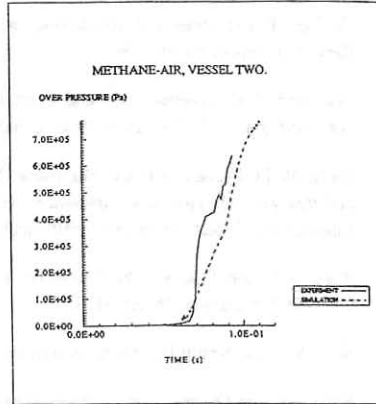


Fig. 2: Explosion in linked vessels - comparison between experiment and simulation for the pressure history in the second vessel.

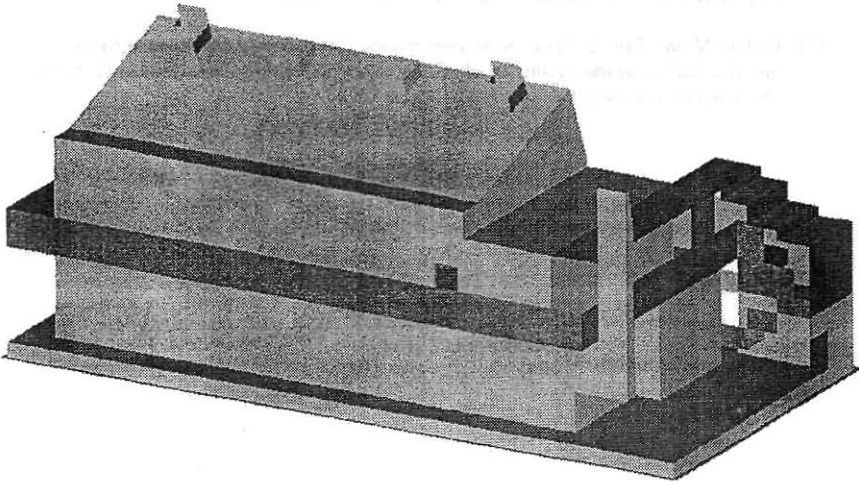


Fig. 3: Semi-confined fire - building geometry.



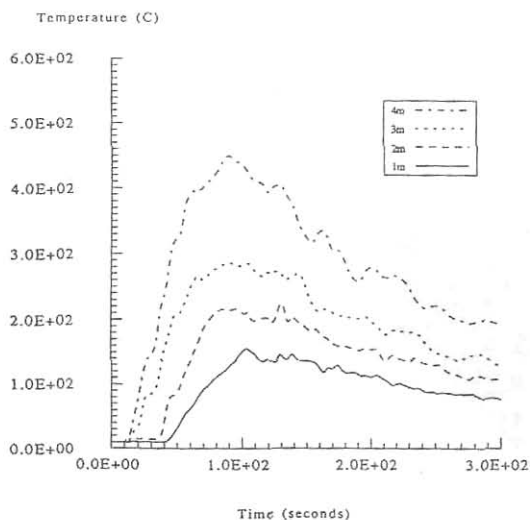


Figure 4: Semi-confined fire - temperature at 4 locations on a vertical rake, as function of time.

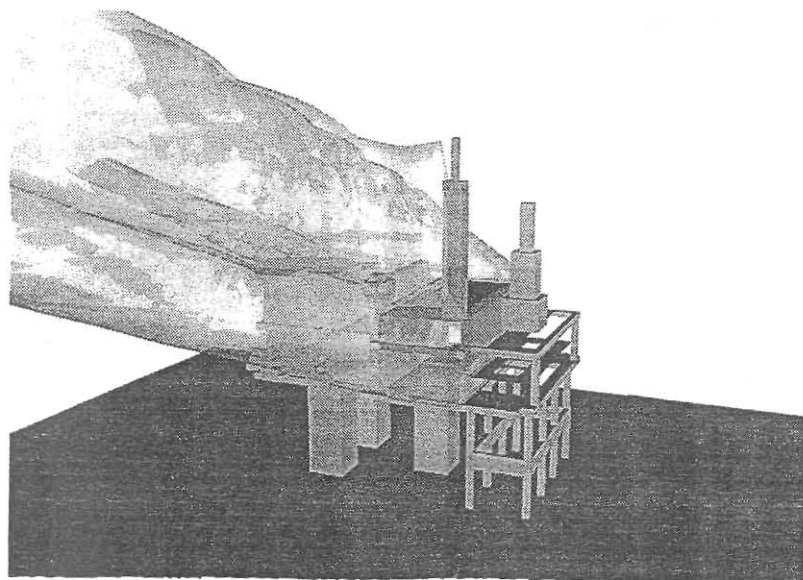


Figure 5: Pool fire on an offshore platform - iso-surface of smoke concentration and temperature contours on the surface of the platform.

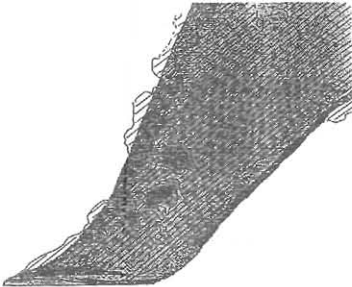


Figure 6: Pool fire - overlay of a video-based image (coarse hatch shaded area denoting sooty regions) and a CFD iso-surface of constant temperature of 300K (continuous grey shading).

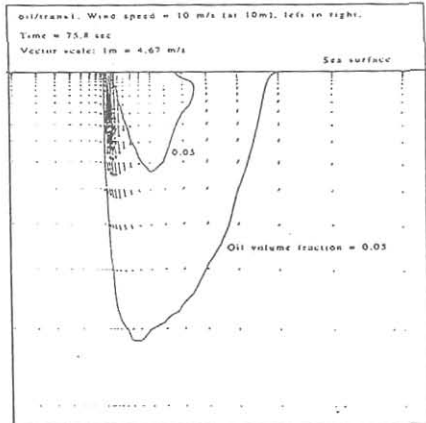


Figure 7: Oil dispersion and burning at sea - velocity vectors and oil concentration (no burning) at  $t=75.8$  sec.

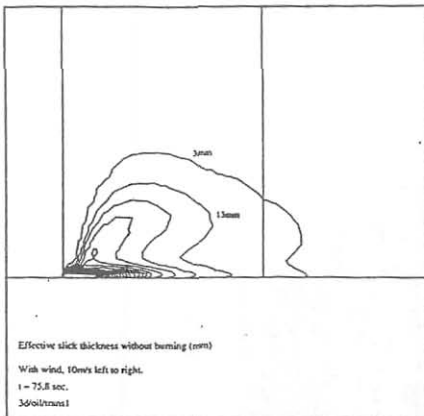


Figure 8: Oil dispersion and burning at sea - effective slick thickness (no burning) at  $t=75.8$  sec. The two vertical lines are 40m apart. The oil enters the sea vertically at 0.

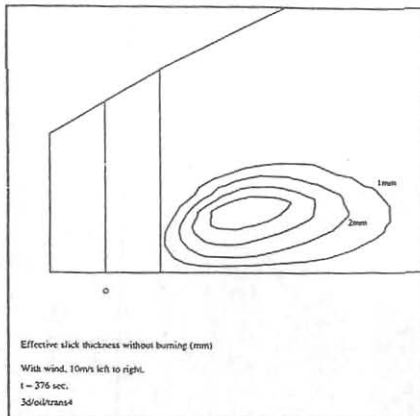


Figure 9: Oil dispersion and burning at sea - effective slick thickness (no burning) at  $t=445.8$  sec.

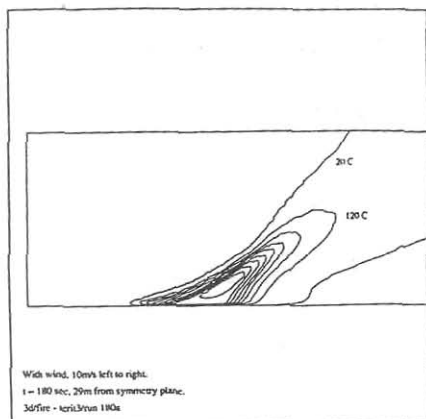


Figure 10: Oil dispersion and burning at sea - fire computation. Temperature contours at  $t=180$ sec, in a vertical plane  $y=29$ m.

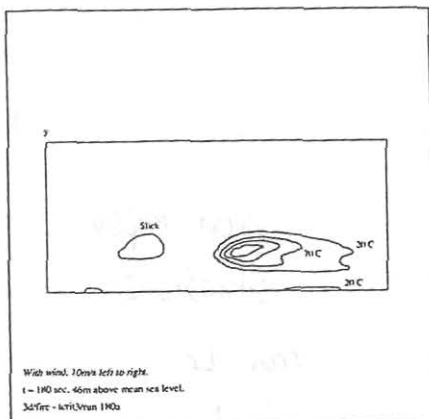


Figure 11: Oil dispersion and burning at sea - fire computation. Temperature contours at  $t=180$ sec, in the horizontal plane  $z=46$ m.

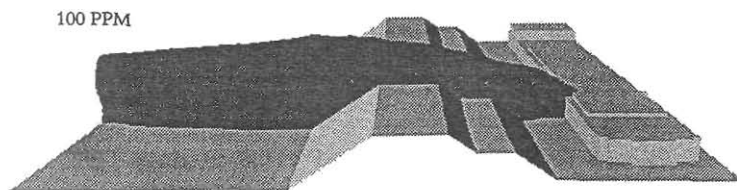


Figure 12: Ammonia dispersion from a barge: ammonia concentration - wind from east.

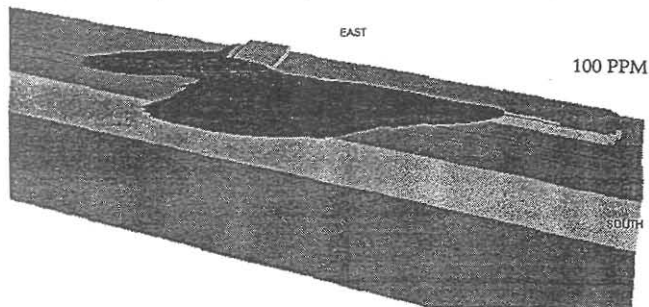


Figure 13: Ammonia dispersion from a barge: ammonia concentration - wind from south-east.

## Paper 8

Full scale module explosion experiments have shown pressures  $> 4.4 \text{ barg}$  for homogeneous gas mixtures throughout module.

These dispersion experiments show that under realistic situations significant homogeneous clouds can be formed, with the cloud size a function of release rate and ventilation rate.