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Gas Explosion Modelling

Comparison between -

ALOHA model

TNT Equivalency Method

CFD (Computerized Fluid Dynamic)

1. INTRODUCTION

1.1. Background

This review is to compare various methods of gas explosion blast wave in order to provide a better estimation to allow better understanding for facility design.
Design of facilities having vapors explosion hazards is a major theme in order to provide a safer environment. The estimating models together with engineering solutions could lead toward better cost effective design.
The core of this review we will compare between the conservative models such as ALOHA & TNT Equivalency Method and the modern CFD (Computerized Fluid Dynamic) model.

1.2. A Description of Gas Explosions

An explosion is the sudden generation and expansion of gases associated with an increase in temperature and an increase in pressure capable of causing structural damage. If there is only a negligible increase in pressure then the combustion phenomena is termed a flash-fire

Gas explosions are generally defined as either confined or unconfined. An explosion in a process vessel or building would be termed as confined. If the explosion is fully confined - i.e. if there is no venting and there is no heat loss, then the over-pressure will be high, up to about eight times higher than the starting pressure. The pressure increase is determined mainly by the ratio of the temperatures of the burnt and unburnt gases. Explosions in confined but un-congested regions are generally characterised by low initial turbulence levels and hence low flame speeds. If the region contains obstacles, the turbulence level in the flow will increase as the fluid flows past the objects, resulting in flame acceleration. If the confining chamber is vented, as is usually the case, then the rate of pressure rise and the vent area become factors that will influence the peak pressure. The rate of pressure rise is linked to the flame speed, which in turn is a function of the turbulence present in the gas.

The over-pressure generated by an unconfined explosion is a function of the flame speed, which in turn is linked to the level of turbulence in the medium through which the flame progresses. As the flame accelerates the pressure waves generated by the flame front begin to coalesce into a shock front of increasing strength. If the explosion occurs in a medium of low initial turbulence, is fully unconfined, and there are no obstacles present then the generated over-pressure is very low. If obstacles are present then expansion-generated flow, created by the combustion, of the unburnt gas passing through the obstacles will generate turbulence. This will increase the burning velocity by increasing the flame area and enhancing the processes of molecular diffusion and conduction, and this will in turn increase the expansion flow which will further enhance the turbulence. This cycle, so called Schelkchkin mechanism, continues generating higher burning velocities and increasing over-pressures.

1.3. Why Model Explosions?

Deflagrations are unwanted events. Models containing physical descriptions of deflagrations are a complement to experiments in risk assessments and/or when designing or assessing mitigating features. The more complex models have the wherewithal to be applied to diverse situations, but must not therefore be assumed to be more accurate.

The effect of an explosion depends on a number of factors, such as maximum pressure, duration of shock wave interaction with structures, etc. These factors in turn depend on a number of variables:

Fuel type

Stoichiometry of fuel

Ignition source type and location

Confinement and venting (location and size)

Initial turbulence level in the plant

Blockage ratios

Size, shape and location of obstacles

Number of obstacles (for a given blockage ratio)

Scale of experiment/plant

The reactivity of fuel has a profound effect on the overpressures generated in a given geometry. The least reactive gas is methane, while acetylene and especially hydrogen give rise to very high pressures.

The stoichiometry of the gas cloud is also important. Lean mixtures produce lower overpressures than rich or stoichiometric mixtures, while slightly rich mixtures yield the highest over-pressures for a given plant layout.

Ignition source type also affects the strength of the explosion; jet-type, or bang-box-type, ignition sources give rise to higher over-pressures than a planar or point source. The location of the ignition is also important, but must be viewed in conjunction with information about the plant geometry, e.g. how confined and/or congested is the plant. Confinement leads to pressure build-up and influences the way the flame front advances through the geometry. Venting is one way of reducing the over-pressure generated by the combustion. Strategically

placed vents can greatly reduce the impact of a deflagration.

Explosions situated in a quiescent environment will generally lead to lower over-pressures than those occuring in turbulent flow environments. This is due to the enhanced burning rate experienced by the flow.

One can define a blockage ratio, which is measure of how congested the plant is. Explosions in plants with large blockage ratios usually yield higher over-pressures than small blockage ratios. However, the size and shape of the obstacles are also important factors to take into account. In general, for a given blockage ratio, many small objects results in higher pressures than larger objects. Furthermore, the location of the obstacles also affects the pressure. The more tortuous route the flame has to travel through the domain, the higher pressure is likely to be produced, due to turbulence enhancement of the burning velocity.

Finally, the scale of experiment/plant is also an important factor. Large-scale experiments generally yield higher pressures than small-scale ones. This makes it difficult to predict, from a small-scale experiment, what the pressures are likely to be in real plants.

Ideally, explosion risks should be considered at the plant design stage, but for various reasons this might not be possible. Unfortunately accidents do happen, but research programmes consisting of experiments and modelling should hopefully result in a better understanding of why the accident happened and how the impact can be minimised or the risk of explosion be mitigated or eliminated completely. In most cases, a great number of scenarios needs to be investigated, which is one justification for developing and using models of varying degrees of complexity.

2. DESCRIPTION AND DISCUSSION OF MODELS

2.1 ALOHA.

As an airborne chemical travels downwind, it mixes with air. A cloud containing a flammable chemical within its flammability limits can ignite if it encounters a spark, flame, or other ignition source. The combustion reaction can propagate away from the source by one of two mechanisms: Deflagration reactions propagate by means of diffusion of reactive species through the cloud. Detonation reactions propagate through a reactive fuel-air mixture by means of a pressure wave that travels at the local speed of sound. Deflagrations propagate more slowly than detonations; however, in either case, the reaction can cause temperatures and pressures within the cloud to increase dramatically. Both detonations and deflagrations can generate pressure waves with sharp onsets and significant overpressures; a pressure wave capable of causing damage to individuals or structures is called a blast wave in ALOHA.

Most vapor cloud combustions are deflagrations that propagate slowly and do not produce blast waves; these are usually referred to as flash fires. For some highly reactive chemicals, the flame speed (the propagation speed) within part of the cloud is accelerated by turbulence caused by obstacles or confinement resulting in a fast deflagration or transition to detonation; either is referred to as an explosion. These events can generate blast waves; usually only a small part of the flammable cloud is involved, so the blast effects are limited. In rare events, a high-power triggering event such as condensed-phase explosive or confined vapor cloud explosion can set off the detonation of the entire flammable cloud. The American Institute for Chemical Engineers (American Institute of Chemical Engineers 1994) estimates that direct initiation of detonation requires approximately one million Joules. The blast wave from the detonation of a large
flammable cloud can have far-reaching effects; they can extend well beyond the area affected by the thermal radiation.

Damage is associated with both the shape and magnitude of the blast wave; both change as the wave travels outward from the reacting cloud. Peak overpressure and impulse are commonly used to characterize the blast wave. Wiekema reports a correlation between lung damage and the combination of overpressure and impulse (Wiekema 1984). Most studies of condensed phase explosions correlate injury with overpressure only. Clancey explained that the relationship
between overpressure and impulse for condensed phase explosions is unique, so a single parameter
is sufficient to describe the blast wave (Institution of Chemical Engineers (Great Britain). North Western Branch. 1982). Injuries and damage to structures from vapor cloud explosions depend on both overpressure and impulse; however, as with condensed phase explosions, most correlations use overpressure only. This

simplification seems to be driven by the lack of data rather than any unique relationship between overpressure and impulse for vapor cloud explosions.

ALOHA uses only peak pressure to characterize the damaging effects associated with a blast wave. Harm can be due to direct effects or indirect effects of the pressure wave. Direct effects include damage to pressure-sensitive organs like ear and lung. Indirect effects can result from glass fragments from broken windows, collapse of buildings, or debris that is accelerated by the blast wave. ALOHA includes three LOCs that quantify indirect and direct effects. Glass windows can shatter at 1 psi over ambient; at 3.5 psi there is a significant risk of eardrum rupture and injuries of serious nature from flying debris; at 8 psi there is significant risk of ear and lung damage and indirect effects from the collapse of unreinforced buildings (Baker 1983).

ALOHA only models combustion reactions. ALOHA estimates the blast wave from unconfined vapor cloud explosions (fast deflagrations and detonations). Unconfined means that the cloud is not entirely or partially bounded by solid walls or ceilings. Confined vapor cloud explosions generally produce more damaging blast waves than unconfined or partially confined explosions.

2.1.1 The Baker-Strehlow-Tang (BST) model

The Baker-Strehlow-Tang (BST) model is the basis for the ALOHA overpressure calculation (Pierorazio et al. 2005); it uses non-dimensional, empirically derived blast curves to predict overpressure. The overpressure is based on the propagation speed of the flame front and the mass of fuel involved in the reaction. The basic principle of this method is that within the vapor cloud there are regions where physical structures can cause an acceleration of the flame front. These areas are characterized by the structure density using a parameter termed congestion. Flame speed is related to the chemical properties of the fuel, the level of congestion, and the nature of the ignition source.

Baker-Strehlow-Tang flame speeds (Mach number). Mach 5.2 is used for deflagration to detonation transition (DDT).

Obstacle Density (Unit less)			**1D Flame Expansion Case (not in use)**	
Low	***Medium***	***High***		
5.2	5.2	5.2	**High**	**Reactivity**
1.03	1.77	2.27	**Medium**	
0.294	1.03	2.27	**Low**	

Obstacle Density (Unit less)			*2D Flam Expansion Case*	
Low	*Medium*	*High*		
0.59	DDT	DDT	*High*	*Reactivity*
0.47	0.66	1.6	*Medium*	
0.079	0.47	0.66	*Low*	

Obstacle Density (Unit less)			*2.5D Flam Expansion Case*	
Low	*Medium*	*High*		
0.47	DDT	DDT	*High*	*Reactivity*
0.29	0.55	1.0	*Medium*	
0.053	0.35	0.5	*Low*	

Obstacle Density			*3D Flam Expansion Case*	
Low	*Medium*	*High*		
0.36	DDT	DDT	*High*	*Reactivity*
0.11	0.44	0.5	*Medium*	
0.026	0.23	0.34	*Low*	

DDT = Deflagration to detonation transition

ALOHA use - Baker-Strehlow-Tang flame speeds (Mach number). Mach 5.2 is used for deflagration to detonation transition (DDT).

	Low congestion	medium congestion	High congestion
High Reactivity	0.36	DDT	DDT
Medium Reactivity	0.11	0.44	0.5
low Reactivity	0.026	0.23	0.34

A reactivity term is used to characterize the chemical properties of the fuel. Reactivity ratings used by Zeeuwen and Wiekema (Zeeuwen and Wiekema 1978) classify reactivity based upon chemical laminar burning velocity in the BST model (Woodward 1998). Low-reactivity chemicals have velocities less than 45 cm/sec. High reactivity applies to those chemicals with burn velocities greater than 75 cm/sec and anything in between is labeled medium reactivity. Some chemicals in the ALOHA database were classified using this criteria; however, most of the flammable chemicals in ALOHA have not been classified. In these cases, ALOHA uses medium reactivity, since few chemicals have laminar burning speeds exceeding 75 cm/sec.

Congestion parameter

A congestion parameter is used to quantify the way small structures within the vapor cloud affect the flame speed. Congestion refers to the density of obstacles that generate turbulence. Obstacles of this nature are generally small, like a shrub, and do not impede the flame front. Larger objects, like a building, can impede the flame front, so they should not be considered obstacles for the purposes of congestion. Greater turbulence allows the flame front to accelerate, thereby generating a more powerful blast wave. The experiments that form the basis for the BST model found the flame speed could be related to area blockage ratio (cross sectional area of the structures divided by area of the cloud) and pitch (distance between rows of structures). The experiments used small structures arranged in regular patterns. Three levels of congestion could be distinguished: low congestion with an area blockage ratio less than 10%; medium congestion with area blockage ratio between 10% and 40%; and high congestion with higher blockage ratios. Extrapolating the laboratory parameters to what is found in an accidental explosion is highly imprecise so ALOHA greatly simplifies the use of congestion. Guidance in ALOHA requires the user to determine whether significant congestion is present. A congested zone is defined as one with so many closely spaced obstacles that it is difficult or impossible to walk through it; for example, pipe racks in industrial facilities and some forested areas where the trees and branches are closely spaced may be characterized as congested zones. To err on the side of caution, congestion defined this way is correlated with the high-congestion flame speed in the BST model.

The source of ignition also affects the flame speed. In ALOHA, the user inputs the ignition source. If the source is designated as a detonation, the model assumes that the triggering

event is of sufficient power to cause the entire reactive cloud to detonate.

ALOHA's method for finding the normalized overpressure as a function of distance from the center of the explosive cloud is based on a set of empirically determined graphs (Pierorazio et al. 2005). BST reported normalized overpressure versus normalized distance from the center of the congested region with a different graph for different flame speeds. To implement these in ALOHA, the graphical data reported by BST were fit to functions of the form purposes of congestion. Greater turbulence allows the flame front to accelerate, thereby generating a more powerful blast wave.

$$\frac{\Delta P}{P_{atm}} = D \; if \; x < x_0,$$
$$else \; \frac{\Delta P}{P_{atm}} = A \cdot B^{1/x} x^C,$$

The experiments that form the basis for the BST model found the flame speed could be related to area blockage ratio (cross sectional area of the structures divided by area of the cloud) and pitch (distance between rows of structures). The experiments used small structures arranged in regular patterns. Three levels of congestion could be

$$\frac{\Delta P}{P_{atm}} = D \; if \; x < x_0,$$

$$else \; \frac{\Delta P}{P_{atm}} = A \cdot B^{1/x} x^C,$$

where ΔP is the maximum overpressure and A, B, C, D, and x_0 are constants. The table

gives values of these constants for various flame Mach numbers.

Curve fit constants for various Mach numbers for use in the BST method.

	Mach 0.2	Mach 0.35	Mach 0.7	Mach 5.2
A	0.0335	0.1041	0.3764	0.2932
B	0.8359	0.8642	0.7439	1.399
C	-1.1192	-1.0568	-1.2728	-1.1591
D	0.065	0.22	0.65	20
x_0	0.35	0.32	0.3	0.16

The normalized distance, x is defined as

$$x = r\left(\frac{P_{atm}}{E}\right)^{1/3},$$

where
P_{atm} is the atmospheric pressure and
r is the distance from the center of the exploding cloud.

The energy contributing to the blast wave is

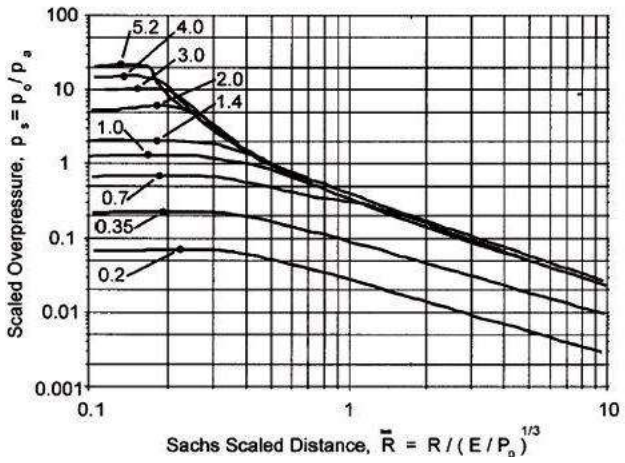
$$E = ref \oplus H_c \oplus Mass\ ,$$

where

ref is a ground reflection factor,

H_C is the heat of combustion of the fuel, and

$Mass$ is the mass of fuel involved in the explosion.



Baker-Stehlow Model for VCE

This curve provides the scaled overpressure as a function of the Sachs scaled distance
Reactivity is classified as low, medium, and high according to the following recommendations of TNO. Methane and carbon monoxide are the only materials regarded as low reactivity, whereas only hydrogen, acetylene, ethylene, ethylene oxide.
And propylene oxide was considered to be highly reactive. All other fuels are classified as medium reactivity. Fuel mixtures are classified according to the concentration of the most reactive component. The Baker–Strehlow pressure curves apply to free air blasts. Since the vapor cloud for

this example is at ground level, the energy of the cloud is doubled to account for the strong reflection of the blast wave.

The ground reflection factor is set to 2 in ALOHA, consistent with the treatment by BST. It accounts for the reflection of the blast wave off the ground. ALOHA's treatment is based on a simplified conceptual model of the explosive cloud. The cloud is treated as a hemisphere at ground level with a uniform concentration. Elevated clouds would have a smaller reflection factor.

The most significant difference between the method in ALOHA and the Baker-Strehlow-Tang model is the method for determining the mass of fuel in the explosion. In the BST method, areas of congestion within a flammable cloud define the mass of fuel contributing to an explosion. The flame front propagates from the point of ignition, accelerates within regions of congestion, and decelerates outside the region of congestion. Only the mass of the fuel within a congested area contributes to the explosion. A flammable cloud emanating from a single release may give rise to as many explosions as there are distinct congested areas. The flame speeds are defined by the levels of congestion within those regions. Outside the congested areas the flame speed is assumed to be so slow that no significant overpressure is generated.

ALOHA uses a different approach for determining the mass of fuel involved in the explosion based on the recommendations of the American Institute for Chemical Engineers (American Institute of Chemical Engineers 1994). AIChE suggests that the BST blast curves can be coupled with an air dispersion model for determining the mass of the explosive cloud, using all the fuel within flammable limits times an efficiency factor. An efficiency factor of 5% to 20% is recommended; ALOHA uses 20%. ALOHA deviates slightly from the AIChE recommendation by using the fuel within a concentration range between the upper explosive limit and 90% of the lower explosive limit. This minor variation was introduced in ALOHA to create another conservative bias in the hazard zone calculation; it was not based on standard practices, theory, or measurement. Gas concentrations above the upper limit are presumed to be too rich, and those below the lower limit too lean, to participate in the explosion. The explosion of the flammable cloud is approximated as a single uniform event; the flame speed is based on the average level of congestion within the cloud.
If the explosion is triggered by a high-power source, termed a hard ignition in ALOHA, or the average level of congestion indicates a transition to detonation, 100% of the mass of the flammable cloud is used and Mach 5.2 is used for the flame speed.

The center of the explosive cloud is equated with the center of mass of flammable cloud in ALOHA. For non-steady-state releases the location of the center and mass of the flammable cloud changes with time. Users may choose the time of ignition; ALOHA then finds the flammable mass and center of the cloud, and generates overpressures as a function of distance.

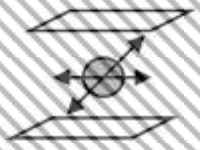
ALOHA can also compute all possible explosions from a single release and show the composite overpressure threat zone if the ignition time is not specified.

This review was conducted by following three approaches. The HSL Sheffield Information Centre was asked to carry out an on-line search seeking information on gas explosion modelling. A number of key words and phrases, as well as a large number of possible authors, were provided

A paper based literature survey was conducted. Relevant reports and papers were collected, the reference lists of which were used to discover further useful sources of information. The survey continued to 'fan out' in this manner, generating a large quantity of useful material. This search has been mainly used to provide the background to this report, but some recent information on certain models was also discovered in the open literature.

Finally, the most recent information on each of the models has been obtained directly from the model developers. This was achieved by sending a standard letter to a number of organisations, inviting comment on the current status and future development of their gas explosion modelling. Further letters were sent to organisations that failed to respond to the original request. Letters were sent to around twenty organisations, over half of which eventually responded to the request for information. Generally, however, the organisations that did reply showed some reluctance to divulge full technical details of their models, most probably due to the increasing commerciality of their operations - either through consultancy or code sales.

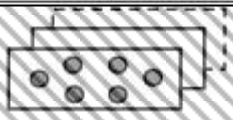
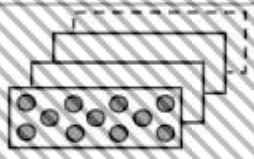
Geometric Considerations for the Baker-Strehlow Vapor Cloud Explosion Model

Dimension	Description	Geometry
3D	"Unconfined volume" almost completely free expansion	
2.5D	Compressor shelters with lightweight roofs; dense pipe racks	Between 3-D and 2-D
2D	Platforms carrying process equipment; space beneath cars; open-sided multistory buildings	
1D	Tunnels, corridors, or sewage systems	

Uncongested for ALOHA calculations

Congested for ALOHA calculations

Confinement Considerations for the Baker-Strehlow Vapor Cloud Expansion Model

Type	Obstacle Blockage Ratio per Plane	Pitch for Obstacle Layers	Geometry
Low	Less than 10%	One or two layers of obstacles	
Medium	Between 10% and 40%	Two to three layers of obstacles	
High	Greater than 40%	Three or more fairly closely spaced obstacle layers	

Uncongested for ALOHA calculations

Congested for ALOHA calculations

Strengths:

Easy to use
Fast
Can handle multi-ignition points

Weaknesses:

Can be over conservative
ALOHA doesn't takes into account some geometrical details, with regards to confinement

2.2. *TNT Equivalency Method*

The TNT equivalency method is based on the assumption that gas explosions in some way resemble those of high charge explosives, such as TNT. However, there are substantial differences between gas explosions and TNT. In the former the local pressure is much less than for TNT detonations. Furthermore, the pressure decay from a TNT detonation is much more rapid than the acoustic wave from a vapour cloud explosion. Nevertheless the model has been used extensively to predict peak pressures from gas explosions. The TNT equivalency model uses pressure-distance curves to yield the peak pressure. One must use a relationship, see below, to find the mass of TNT equivalent to the mass of hydrocarbon in the cloud.

W_{TNT} 10 W_{HC} , [kg] (1)

Where W_{TNT} is the mass of TNT, W_{HC} is the actual mass of hydrocarbons in the cloud, and is a yield factor (0.03-0.05) based on experience. The factor 10 represents the fact that most hydrocarbons have ten times higher heat of combustion than TNT. In the original TNT equivalency model no consideration was taken of the geometry and therefore it is recommended that this model should not be used, Bjerketvedt, Bakke and van Wingerden (1997).

A TNT equivalency model which does take geometry effects into account has been proposed, Harris and Wickens (1989). Results from experiments formed the basis for the new formulation. The yield factor was increased to 0.2 and the mass of hydrocarbon in stoichiometric proportions was to correspond to the mass of gas in the severely congested region of the plant. For natural gas the mass of TNT can be arrived at using

$W_{TNT} = 0.16\ W_{eff}$, [kg] (2)

where $V_{eff} = \min (V_{con}, V_{cloud})$ is the total volume of the congested region and $_{Vcloud}$ is the total volume of the gas cloud. The equation will hold for most hydrocarbons. It is recommended that the TNT equivalency model should not be used.

Pressure Rise from a Confined Explosion

$(P_{max})/P_a = (T_{ad}/T_a)$

$P_{max} = (T_{ad}/T_a)\ P_a$

Where,

P_a = initial atmospheric pressure (kPa)
T_a = ambient temperature (K)
T_{ad} = adiabatic flame temperature (K)

2.3. CFD Models

2.3.1. Introduction

Computational Fluid Dynamics (CFD) models find numerical solutions to the partial differential equations governing the explosion process. The Navier-Stokes equations, which govern the fluid flow, and the sub-models used to represent the terms which are not modelled exactly. The numerical solutions are generated by discretizing the solution domain (in both space and time). The conservation equations are applied to each of the sub-domains formed by the discretization process, generating a number of coupled algebraic equations that are normally solved by an iterative procedure.

Solutions obtained with CFD codes contain a great wealth of information about the flow field, i.e. velocities, pressure, density, species concentrations, etc. Surface pressure data can be used for structural analysis. CFD is widely applicable and can be used in many different disciplines - from designing aeroplanes, cars or artificial heart valves, to weather forecasting and environmental modelling. CFD simulations can offer insight into the flow behaviour in situations where it is impractical or impossible to carry out experiments. In principle, it is possible to try out many different scenarios, with little extra effort. CFD and experiments should be viewed as complementary means of investigating flow situations. It is vitally important that the sub-models used are properly validated against well-controlled, well-defined and repeatable experiments. If the models have not been validated, confidence in the results obtained from calculations with CFD codes must be low, and the results used with prudence, if at all. The importance of solving the right problem, i.e. using the correct geometry, correct initial and boundary conditions, can not be over emphasised. CFD codes are immensely powerful and useful tools, if applied correctly.

The main drawbacks associated with the use of CFD are caused by the limitations imposed by the available computing hardware, for example it is currently impractical (if not impossible) to simulate exactly a turbulent combusting flow. Hence, sub-models of combustion and turbulent transport have been developed that simplify the calculation process. Small-scale (relative to the explosion domain) objects may cause significant over-pressure generation in a gas explosion, due to the turbulence generated.
The rate of progress in model development in the field has been relatively slow. Turbulence remains a highly active topic of research. The mathematical understanding of the subject is improving, but there are still a number of issues which have not been fully resolved, i.e. transition from laminar to turbulent flow. Furthermore, the process of incorporating the new findings into the existing turbulence models has been slow. This is to some extent due to the fact that most of these models are relatively crude approximations of reality and can therefore not easily accommodate the mechanisms involved. The first papers discussing second moment closure modelling appeared in the early 1970's. In principle, second moment closures should be more general that the simpler turbulence models, Models of that

complexity should able to better represent many different types of flows. But thirty years on, Reynolds stress transport models are still not applied routinely. The implementations of Reynolds stress models in the currently available commercial CFD codes lack one of the most important properties to industry, namely robustness.

In fairness, some of the outstanding issues are to do with numerical aspects, i.e. discretisation of the transport equations, etc., rather than to do with the numerical modelling. It seems unlikely that fully simulating a turbulent combusting flow in a real plant - with all its associated time and length scales, and involving a great number of obstacles and other configurational complexities, will be possible for several decades, judging by the current rate of progress. However the rapid development of faster processors with more random access memory, and parallel processing - but which might require rewriting of parts of the CFD codes to take full advantage of massively parallel architecture, may go some way to alleviate matters.

2.3.2 PHOENICS

2.3.2.1 PHOENICS is a general-purpose software package which uses the techniques of CFD (*i.e.* Computational Fluid Dynamics) to predict quantitatively:

- PHOENICS has been continuously marketed, used and developed since 1981. Many, but surprisingly not all (*e.g.* the parabolic option) of its original features have found their way into competitive codes; but its newer ones (*e.g.* In-Form, MUSES, IMMERSOL) remain unique.
- PHOENICS is also used as the 'computational engine' of **special-purpose** software packages, whether its own, such as FLAIR for heating, ventilating and air-movement simulation, or within other company's packages, such WINDSIM, for wind-farm simulation.

2.3.2.2 **Physical and mathematical content of PHOENICS**

PHOENICS has all the features which are common to commercial CFD codes; indeed it pioneered them. Since the present document is an overview rather than a text-book, it has been judged sufficient here simply to list the conventional features, under two headings, namely: physical, and mathematical.

Thereafter some of the less conventional features of PHOENICS will be given more attention.

(a) Physical

- PHOENICS simulates flow phenomena which are:
    - laminar or turbulent
    - compressible or incompressible
    - steady or unsteady

    - chemically inert or reactive
    - single- or multi-phase
    - in respect of thermal radiation:
        - transparent
        - participating by way of absorption and emission
        - participating by way of scattering.

- The space in which the fluid flows may be:
    - empty of solids, or
    - wholly or partially filled by finely-divided solids at rest (as in 'porous-medium' flows), or
    - partially occupied by solids which are not small compared with the size of the local computational cells.
- In the latter two cases, the solids may interact thermally with the solids (that is to say that PHOENICS can handle 'conjugate heat transfer').
- Such immersed solids can also participate in radiative heat transfer.
- The thermally and mechanically-induced stresses and strains in the immersed solids can also be computed by PHOENICS.
- The thermodynamic, transport (including radiative), chemical and other properties of the fluids and solids may be of arbitrary complexity.

(b) Mathematical

- The equations solved by PHOENICS are those which express the balances of:
    - mass
    - momentum
    - energy
    - material (ie chemical species)
    - other conserved entities (e.g. electrical charge)

  over discrete elements of space and time, i.e. 'finite volumes' known as 'cells'.
- The cells are arranged in an orderly (i.e. "structured") manner in a grid which may be:

  - cartesian,
  - cylindrical-polar, or
  - "body-fitted", i.e. arbitrarily curvi-linear,

  and which may be segmented into distinct "blocks".
- These equations express the influences of:
  - diffusion (including viscous action and heat conduction),
  - convection,
  - variation with time,
  - sources and sinks.
- In order to reduce the numerical errors which may result from the unsymmetrical nature of the convection terms, PHOENICS can make use of a large variety of 'higher-order schemes', including QUICK, SMART, Van Leer, and many others.
- The dependent variables of these equations are thus:
  - mass or volume fraction,
  - velocity and pressure,
  - temperature or enthalpy,
  - concentration,
  - electrical charge or other conserved property.
- The mass and momentum equations are solved in a semi-coupled manner by a variant of the well-known SIMPLE algorithm.
- Because the whole equation system is non-linear, the solution procedure is **iterative**, consisting of the steps of:
  - computing the imbalances of each of the above entities for each cell;
  - computing the coefficients of linear(ised) equations which represent how the imbalances will change as a consequence of (small) changes to the solved-for variables;
  - solving the linear equations;
  - correcting the values of solved-for variables, and of auxiliary ones, such as fluid properties, which depend upon them:

- repeating the cycle of operations until the changes made to the variables are sufficiently small.

- Various techniques are used for solving the linear equations, including:
  - tri-diagonal matrix algorithm
  - (a variant of) Stone's 'Strongly Implicit Algorithm',
  - conjugate-gradient and conjugate-residual solvers.

2.3.2.2 Simulation of multi-phase flow in PHOENICS

"Multi-phase flows" are those involving, to name but a few examples:-

- steam **and** water in a boiler,
- air **and** sand in a desert storm,
- fuel droplets **and** combustion gases in an engine,
- a layer of oil, floating on the surface of a river.

PHOENICS was the first general-purpose computer code to be able to simulate multi-phase flows; and it is still capable of doing so more effectively, and in a greater variety of ways, than most of its competitors.

2.3.2.4 Turbulence models in PHOENICS

The flows which PHOENICS is called upon to simulate are, more often than not, **turbulent**, by which is meant that they exhibit near-random fluctuations, the time-scale of which is very small compared with the time-scale of the mean-flow, and of which the distance scale is small compared with the dimensions of the domain under study.

Since the beginning of the practice of computational fluid dynamics, in the 1960's, the impracticability (or, more precisely, the prohibitive expense) of predicting these fluctuations has resulted in the invention of "turbulence models" which represent, to some extent, their results.

Satisfactoriness

A broad-brush summary of the satisfactoriness of the most-widely-used turbulence models is:

- for predicting time-average hydrodynamic phenomena and the macro-mixing of fluids marked by conserved scalars, the models are "not bad"; but

- for the simulation of micro-mixing, which is essential if chemical-reaction rates are to be predicted, they are very poor indeed; and
- the most distressing aspect of the last-mentioned point is that it is not sufficiently recognised by the users of the models.

Turbulence models in PHOENICS

PHOENICS is particularly rich in turbulence models, as can be seen from the relevant .

Two of these are of special interest, because they are unique to PHOENICS, namely:

a. The LVEL model is most useful in circumstances in which many solids are immersed in the fluid, making conventional "two-equation" models impractical.

   It handles the complete range of Reynolds number smoothly; and it contains its own unique and simple method for calculating the distances to and between walls.

b. possesses more radical novelty; for it provides a direct means of computing the quantities of practical importance, so supplanting the conventional indirect means.

2.3.2.5 Radiative-heat-transfer models in PHOENICS

PHOENICS is supplied with several means of computing thermal radiation, A method which is unique to PHOENICS, and is especially convenient when radiating surfaces are so numerous, and variously arranged, that the use of the view-factor-type model is impractically expensive, is IMMERSOL.

This method is:

- computationally inexpensive;
- capable of handling the whole range of conditions from optically-thin (ie transparent) to optically-thick (ie opaque) media;
- mathematically exact when the geometry is simple; and
- never grossly inaccurate even when it is not,

2.3.2.6 Variables

Variables may be thought of as being:

- dependent - the subject of a conservation equation
- auxiliary - constant, or derived from an algebraic expression.

In each case, they can be further subdivided into scalar and vector quantities:

- Dependent:

  Scalars:

  - Pressure
  - Temperature
  - Enthalpy
  - Mass fractions
  - Volume fractions
  - Turbulence quantities
  - Various potentials

  Vectors:

  - Velocity resolutes
  - Radiation fluxes
  - Displacements

- Auxiliary:

  Scalars:

  - Density
  - Viscosity
  - Conductivity
  - Diffusivity
  - Specific heat
  - Thermal expansion coefficient
  - Inter-fluid transport
  - Absorptivity
  - Compressibility

Vectors:

  - Various non-isotropic properties

- Gravity forces
- Other body forces

The quantities defining the problem geometry can also be divided into scalar and vector categories:

- Geometric:

Scalars:

- Cell volumes
- Volume porosity factors
- Inter-fluid surface area per unit volume

Vectors:

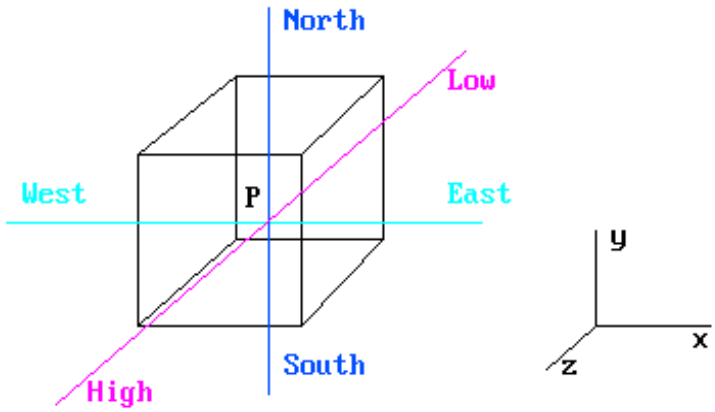
- Cell center coordinates
- Cell corner coordinates
- Center to center distances
- Cell surface areas
- Cell area porosities

2.3.2.7 Storage

The distinction between scalar and vector is important, because each is stored at a different location in space:

- Scalars - These are stored at the center points of six-sided cells, with values supposed to be typical of the whole cell.
- Vectors - These are stored at the center points of the six cell faces.

Nomenclature - A compass-point notation is used, as shown below



P = Cell center

N,S,E,W,H,L = Neighbour-cell centers

S -> N = Positive IY

W -> E = Positive IX

L -> H = Positive IZ

T = Cell center at previous time step

An array of cells with the same IZ is referred to as a SLAB.

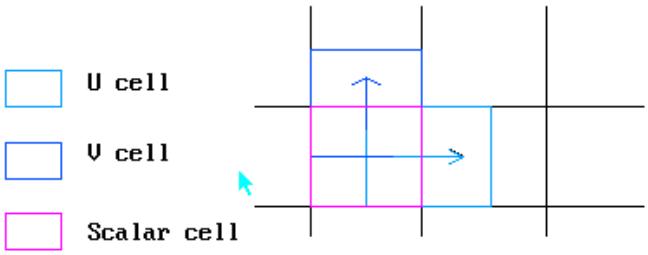
Steady or Transient

Steady-State Problems - PHOENICS can proceed directly to the steady-state solution. It is not necessary to march through time to reach the steady state.

Transient Problems - PHOENICS can cope with constant and variable time steps. The time step size can be a function of time.

2.3.2.8 Grids

Vector quantities are computed by reference to cells which are staggered with respect to the scalar cells.



3 velocities and 1 scalar share the same cell index (IX,IY,IZ).

Any scalar or vector quantity can only be referenced by a unique (IX,IY,IZ) index. Thus the velocity on the West face of the cell P above 'belongs' to the West scalar cell.

Types of Grid

PHOENICS grids are structured - cells are topologically Cartesian brick elements.

PHOENICS grids may be :

- Cartesian
- Cylindrical-polar
- Body fitted, orthogonal or non-orthogonal

In all cases, the grid distribution can be non-uniform in all coordinate directions.

For cylindrical-polar coordinates, the following orientation is used:

- X (or I) is always the angular direction
- Y (or J) is always the radial direction
- Z (or K) is always the axial direction

This modern CFD sets of codes uses an automatic Grid / Mesh sizing by the auto-mesher according to these:

1. The maximum cell size is not allowed to exceed a set fraction (0.05 by default) of the domain size.

2. The ratios between the sizes of the first cell in the current region and the last cell in the previous region, and the last cell in the current region and the first cell in the next region, are not allowed to exceed a set limit (1.5 by default).

3. If the ratios are exceeded, the number of cells in that region is increased, and the spacing is set according to a geometrical or power-law progression using a set expansion ratio (geometrical 1.2 by default), until either the ratio criterion is satisfied at both ends of the region, or the cells at both ends are below a set minimum fraction (0.005 by default) of the domain size.

Where there is an INLET object on the edge of the domain, the auto-meshing will assume that grid is required in that direction, even if there is only one region.

After the meshing an adjustment was made before a final run was made.

The adjustment include refining cell number and the use of the power-law or geometrical expansions to reduce the change in grid-size between regions. This assists convergence of the Earth solver. With the auto-meshing turned on, this is controlled by reducing the minimum cell size and adjusting the maximum size ratio. Reducing both these values will act to reduce the rate of change of grid size across region boundaries, but also increase the number of cells.

2.3.2.9 The Balance Equation

Basic form

The basic balance, or conservation equation is just:

Outflow from cell - Inflow into cell = net source within cell

The quantities being balanced are the dependent variables from the earlier panel:

- mass of a phase
- mass of a chemical species
- energy

- momentum
- turbulence quantities
- electric charge etc.

The terms appearing in the balance equation are:

- Convection (i.e., directed mass flow)
- Diffusion (i.e., random motion of electrons, molecules or larger structures e.g., eddies)
- Time variation (i.e., directed motion from past to present - accumulation within a cell)
- Sources (e.g., pressure gradient or body force for momentum, chemical reaction for energy or chemical species)

2.3.2.10 The Generalized Form

The single phase conservation equation solved by PHOENICS can be written as:

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial}{\partial x_k}\left(\rho U\phi - \Gamma_\phi \frac{\partial\phi}{\partial x_k}\right)=S_\phi$$

where: f - the variable in question

r - density

U - vector velocity

Γ_ϕ - the diffusive exchange coefficient for f

S_ϕ - the source term

2.3.2.11 Particular Forms

Particular examples are:

$\phi = u, v, w$

$\Gamma_\phi = \rho(\nu_T + \nu_L)$

$S_\phi = -\frac{\partial p}{\partial x_k} + \text{gravity} + \text{friction} + \ldots$ Momentum

$$\phi = h$$

$$\Gamma_\phi = \rho\left(\frac{\nu_t}{Pr_t} + \frac{\nu_l}{Pr_l}\right)$$

$$S_\phi = -\frac{Dp}{Dt} + \text{heat sources} + \ldots$$ Enthalpy

$$\phi = 1$$

$$\Gamma_\phi = 0$$

$$S_\phi = 0 + \text{boundary sources}$$ Continuity

where ν_t, ν_l are the turbulent and laminar viscosities, and Pr_t, Pr_l are the turbulent and laminar Prandtl/Schmidt Numbers.

2.3.2.12 Numerical solution

The balance equations cannot be solved numerically in differential form. Hence, PHOENICS solves a finite-volume formulation of the balance equation.

The FVE's are obtained by integrating the differential equation over the cell volume.

Interpolation assumptions are required to obtain scalar values at cell faces and vector quantities at cell centers.

No Taylor series expansion or variational principle is used.

2.3.2.12 Finite Volume Form

After integration, the FVE has the form:

$$a_P\phi_P = a_N\phi_N + a_S\phi_S + a_E\phi_E + a_W\phi_W + a_H\phi_H + a_L\phi_L + a_T\phi_T + \text{source terms}$$

where:

$$a_P = a_N + a_S + a_E + a_W + a_L + a_H + a_T$$ (by continuity)

The neighbour links, the a's, have the form

$$\text{area} \times \text{velocity} \times \text{density} + \frac{\text{area} \times \text{exchange - coefficient}}{\text{distance}} + \frac{\text{volume} \times \text{density}}{dt}$$

convection diffusion transient

2.3.2.13 Correction Form

The equation is cast into correction form before solution.

In correction form, the sources are replaced by the errors in the real equation, and the coefficients may be only approximate. The corrections tend to zero as convergence is approached, reducing the possibility of round-off errors affecting the solution.

The neighbor links:

- Increase with inflow velocity, cell area, fluid density and transport coefficient
- Decrease with internodal distance
- Are always positive.

2.3.2.14 Boundary Conditions

Boundary Conditions can be:

- Fixed value
- Fixed flux
- Linear
- Non-linear

2.3.2.15 General form

Boundary Conditions are represented in PHOENICS as linearized sources for cells adjacent to boundaries:

$$S_\phi = a_{BC}\left(\phi_{BC} - \phi_P\right)$$

a_{BC} is termed the COEFFICIENT.

ϕ_{BC} is termed the VALUE.

a_{BC} is added to a_P, and $a_{BC}\phi_{BC}$ is added to the RHS of the equation for ϕ_P

.

$$\phi_P = \frac{\sum a_k \phi_k + a_{BC}\phi_{BC}}{a_P + a_{BC}}$$

2.3.2.16 Particular forms

For a fixed value boundary, a_{BC} is made very big. The effect is:

$$\phi_P = \frac{\sum a_k \phi_k + a_{BC}\phi_{BC}}{a_P + a_{BC}}$$

$$\phi_P = \frac{\text{very small number} + a_{BC}\phi_{BC}}{\text{very small number} + a_{BC}}$$

$$\phi_P = \phi_{BC}$$

For a fixed flux boundary, a_{BC} is made very small, and $a_{BC}\phi_{BC}$ is set to the required flux.

$$\phi_P = \frac{\sum a_k \phi_k + \text{tiny}\dfrac{\text{source}}{\text{tiny}}}{a_P + \text{tiny}}$$

$$\phi_P = \frac{\sum a_k \phi_k + \text{source}}{a_P}$$

Linear and non-linear conditions can be set by appropriate prescription of a_{BC} and ϕ_{BC}

3. Scenario.

3.1 In order to compare the models, we have chosen simple scenarios which would emphasize the differences between the models.

3.2 The scenario that was chosen is:

- High pressure Methane leak out of 1" pipe end.
- The gas cloud ignites and explodes after 1 minute.
- The leak source was located in an open area and in a semi enclosure concrete bunker.

3.3 ALOHA.

3.3.1 General.

CHEMICAL DATA:

Chemical Name: METHANE Molecular Weight: 16.04 g/mol
PAC-1: 2900 ppm PAC-2: 2900 ppm PAC-3: 17000 ppm
LEL: 50000 ppm UEL: 150000 ppm
Ambient Boiling Point: -161.7° C
Vapor Pressure at Ambient Temperature: greater than 1 atm
Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 1 meters/second from E at 3 meters
Ground Roughness: open country Cloud Cover: 5 tenths
Air Temperature: 20° C Stability Class: F
No Inversion Height Relative Humidity: 50%

SOURCE STRENGTH:

Flammable gas escaping from pipe (not burning)
Pipe Diameter: 1 inches Pipe Length: 20 meters
Unbroken end of the pipe is connected to an infinite source
Pipe Roughness: smooth Hole Area: 0.79 sq in
Pipe Press: 250 atmospheres Pipe Temperature: 20° C
Release Duration: ALOHA limited the duration to 1 hour
Max Average Sustained Release Rate: 376 kilograms/min
(averaged over a minute or more)
Total Amount Released: 22,577 kilograms

3.3.2 Uncongested (Easy to walk through).

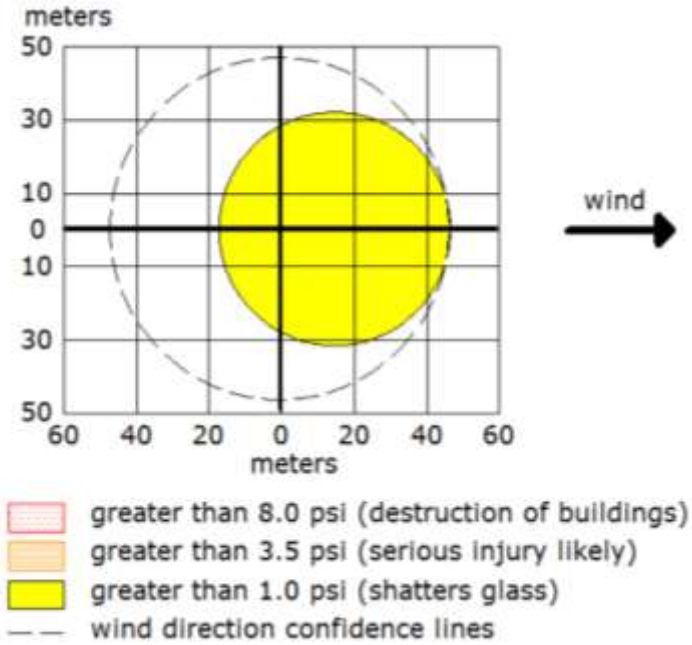
THREAT ZONE:

Threat Modeled: Overpressure (blast force) from vapor cloud explosion
Time of Ignition: 1 minutes after release begins
Type of Ignition: ignited by spark or flame
Level of Congestion: uncongested
Model Run: Heavy Gas
Explosive mass at time of ignition: 80.7 kilograms
Red : LOC was never exceeded --- (8.0 psi = destruction of buildings)
Orange: LOC was never exceeded --- (3.5 psi = serious injury likely)
Yellow: LOC was never exceeded --- (1.0 psi = shatters glass)

3.3.3 Congested (Not easy to walk through).

THREAT ZONE:

Threat Modeled: Overpressure (blast force) from vapor cloud explosion
Time of Ignition: 1 minutes after release begins
Type of Ignition: ignited by spark or flame
Level of Congestion: congested
Model Run: Heavy Gas
Explosive mass at time of ignition: 80.7 kilograms
Red : LOC was never exceeded --- (8.0 psi = destruction of buildings)
Orange: LOC was never exceeded --- (3.5 psi = serious injury likely)
Yellow: 47 meters --- (1.0 psi = shatters glass)



3.4 CFD.

3.4.1 In order to use the CFD models, the initial and boundary conditions should be set. The initial conditions such as environment temperature, pressure and wind were put into to the CFD model. The initial pressure of the exploding body was calculated using the TNT equivalent model using the amount of gas calculated by the ALOHA in order to equalize the initials.

3.4.1.1 TNT equivalent to calculate the initial over pressure.

The calculations are based on principles developed in the SFPE Handbook of Fire Protection Engineering using the NRC spreadsheet chapter 15 'ESTIMATING PRESSURE INCREASE AND EXPLOSIVE ENERGY RELEASE ASSOCIATED WITH EXPLOSIONS'

EXPLOSIVE ENERGY RELEASE ASSOCIATED

Version 1805.1

INPUT PARAMETERS

Adiabatic Flame Temperature of the Fuel (T_{ad})	1173	°C
Heat of Combustion of the Fuel (ΔH_c)	50030	
Yield (α) See Note	100.00	%
Mass of Flammable Vapor Release (m_F)	376.00	kg
Ambient Air Temperature (T_a)	25.00	°C
Initial Atmospheric Pressure (P_a)	101.35	kPa

FUEL FLAMMABILITY DATA

Fuel	Adiabatic Flame Temperature T_{ad} (°C)	Heat of Combustion ΔH_c (kJ/kg)
Methane	1173	50,030
Reference: SFPE Handbook of Fire Protection Engineering, 2nd Edition, 1995, Page 1-86.		

METHOD OF ZALOSH

Reference: SFPE Handbook of Fire Protection Engineering, 2nd Edition, 1995, Page 3-312.

Pressure Rise from a Confined Explosion

$$(P_{max})/P_a = (T_{ad}/T_a)$$

$$P_{max} = (T_{ad}/T_a)\, P_a$$

Where,

P_{max} = maximum pressure developed at completion of combustion (kPa)
P_a = initial atmospheric pressure (kPa)
T_{ad} = adiabatic flame temperature (K)
T_a = ambient temperature (K)

P_{max} = 491.79 kPa 71.33 psi

Blast Wave Energy Calculation

$$E = \alpha\, \Delta H_c\, m_F$$

Where,

E = blast wave energy (kJ) [E is the Trinitrotoluene (TNT) equivalent energy]
α = yield (a is the fraction of available combustion energy participating in blast wave generation)
ΔH_c = heat of combustion (kJ/kg)
m_F = mass of flammable vapor release (kg)

E = 18811280.00 kJ

TNT Mass Equivalent Calculation

$$W_{TNT} = E/4500$$

Where,

W_{TNT} = weight of TNT (kg)
E = explosive energy release (kJ)

W_{TNT} =	**4180.28**	**kg**	**9215.95**	**lb**

Pressure Rise from a Confined Explosion

$P_{max} = (T_{ad}/T_a) P_a$

P_{max} =	**491.79**	**kPa**	**71.33**	**psi**

Blast Wave Energy

$E = \alpha \Delta H_c m_F$

E =	**18811280.00**	**kJ**	**17816163.29**	**Btu**

TNT Mass Equivalent

$W_{TNT} = E/4500$

W_{TNT} =	**4180.28**	**kg**	**9215.95**	**lb**

3.4.1.2 CFD boundary

The CFD code in use is PHOENIX Flair by CHAM UK is a modern CFD sets of codes uses an automatic Grid / Mesh sizing by the auto-mesher following these guidelines:

- The maximum cell size is not allowed to exceed a set fraction (0.05 by default) of the domain size.
- The ratios between the sizes of the first cell in the current region and the last cell in the previous region, and the last cell in the current region and the first cell in the next region, are not allowed to exceed a set limit (1.5 by default).

- If the ratios are exceeded, the number of cells in that region is increased, and the spacing is set according to a geometrical or power-law progression using a set expansion ratio (geometrical 1.2 by default), until either the ratio criterion is satisfied at both ends of the region, or the cells at both ends are below a set minimum fraction (0.005 by default) of the domain size.

  Where there is an INLET object on the edge of the domain, the auto-meshing will assume that grid is required in that direction, even if there is only one region.

  After the meshing an adjustment was made before a final run was made.

  The adjustment include refining cell number and the use of the power-law or geometrical expansions to reduce the change in grid-size between regions. This assists convergence of the Earth solver. With the auto-meshing turned on, this is controlled by reducing the minimum cell size and adjusting the maximum size ratio. Reducing both these values will act to reduce the rate of change of grid size across region boundaries, but also increase the number of cells.

The model settings are as follows:

DOMAIN SIZE:

X - 400 m

Y - 400 m

Z – 200 m

COMPUTATIONAL GRID

NX – 60 cells

NY – 68 cells

NZ – 21 cells

The model settings are as follows:

BOUNDARY CONDITIONS

Side and top outlets from the domain: fixed pressure boundary condition with atmospheric pressure

Initial pressure of explosion 4.91 brag.

Initial Temperature of explosion 1500°C

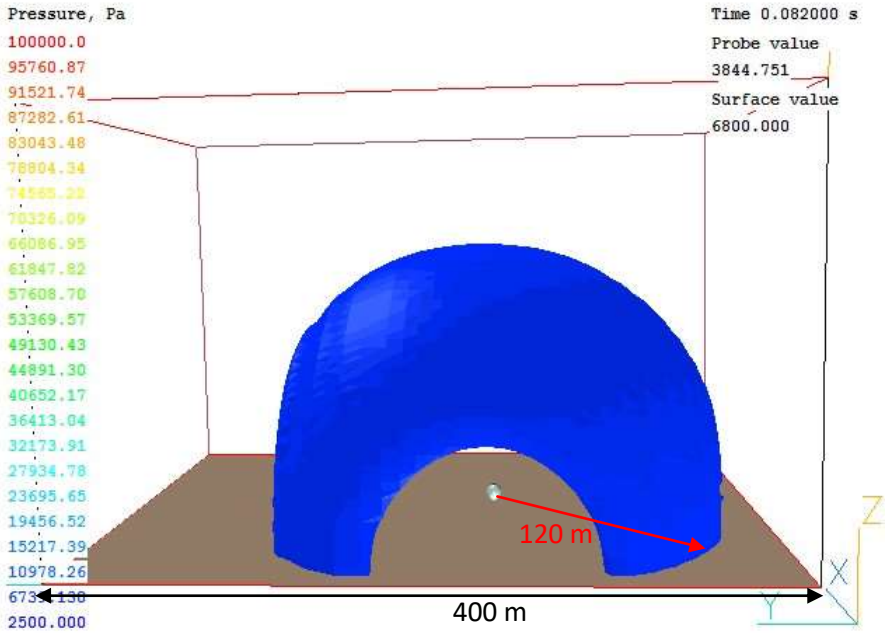
Explosion duration 0.01s

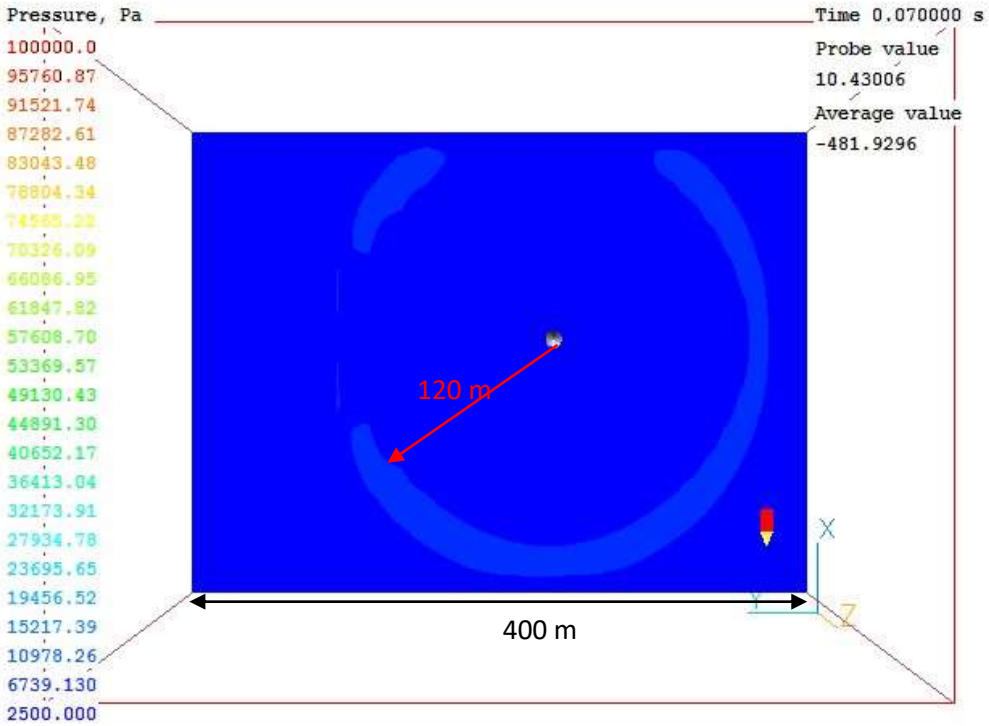
Calculation duration – 0.6 s (0.001 s intervals)

Ground plane – plate object .

3.4.2 Outdoors explosion without protection walls .

3.4.2.1 1 psi contour .

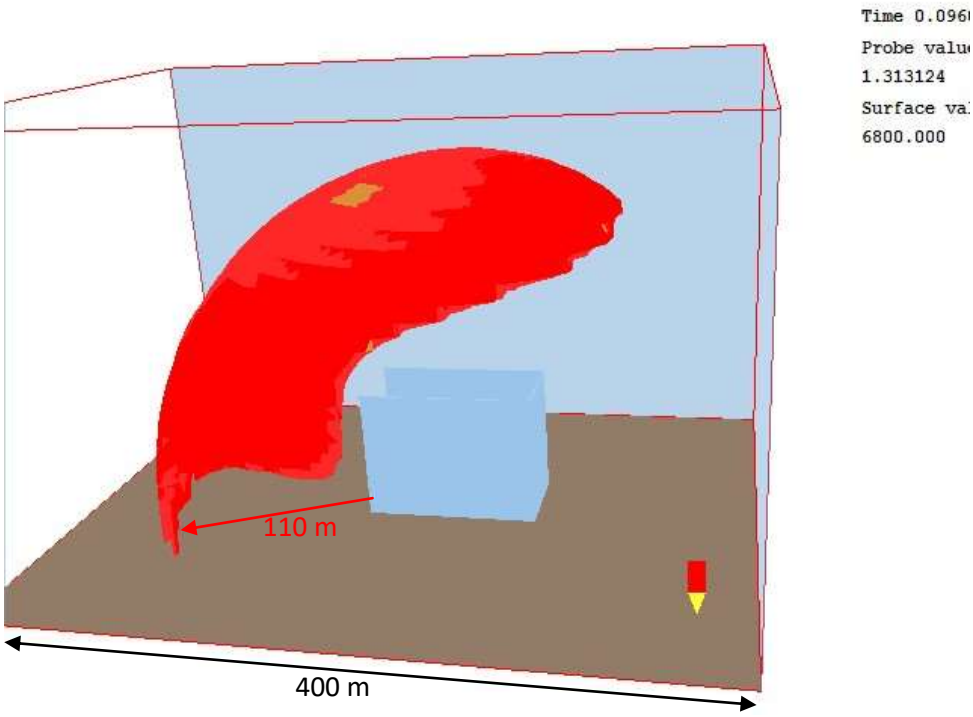




3.4.2.1.1 Animation for Blast wave CFD simulation without walls

3.4.2 Outdoors explosion with protection walls .

3.4.2.1 1 psi contour after 0.082 s



3.4.2.1.1 Animation for Blast wave CFD simulation with walls

4. DISCUSSION

3.1. Overview of Model Constraints

The empirical model constraints are twofold. Firstly the geometrical representation is quite crude, and secondly, the relative lack of physics incorporated in these models means that they have to be calibrated for every fuel. One of the models, the TNT equivalency model, even assumes that gas explosions behave like TNT explosions, which is not the case. It is necessary to make assumptions about the explosion source strength and degree of confinement, etc., when using some of the models, leading to a range of possible answers, i.e. uncertainties. There are guidelines for how to estimate source strength and confinement, but it is inevitably a much simplified approach. These approaches are open to abuse by inexperienced users or extrapolation beyond bounds of applicability, but many of constraints forced by use of a simple method designed to generate answers with the minimum of effort.

The phenomenological models contains more physics than the empirical models. Moreover, it is still necessary to carry out calibrations for all fuels of interest. The geometry is not represented in as a great detail as in the CFD codes reviewed in the present report, though one of the codes, CLICHE, calculates its input parameters from an obstacle database, which in principle allows a more accurate representation. There is also uncertainty introduced by non-unique obstacle representation - the choice of obstacle representation dependent on the experience of the user.

There are several fundamental constraints imposed on the CFD models discussed in this report.

The first constraint applies to the representation of the modelled geometry. (This is not applicable to the empirical and the phenomenological model type, as these attempt no detailed representation of the actual geometry.) Desktop computers presently have only a limited amount of memory, the maximum capacity being of the order 10^9 bytes. However, the latest desktop PC's, even with more than 1 Gb of random access memory, are becoming very affordable, and offer fast processor speeds, compared to many (more expensive) workstations. It is also possible to reduce the amount of memory required (per processor) by partitioning the mesh into a number of smaller parts, e.g. use a parallelized version of the CFD code. Clusters of PC's, i.e. Beowulf clusters, running the Linux operating system, are now making parallel computing affordable. In light of this, memory constraints might become less of an issue in the next decade.

Experience has shown that each finite volume used by a CFD code requires around 10^3 bytes of computer memory. Hence, the maximum number of finite volumes available to represent a geometry on a poweful desktop PC is around 10^6. In three dimensions this would allow approximately 100 volumes in each co-ordinate direction, equating to equal sized cells of around 0.1 to 1.0 m per side for typical process plant. Many of the objects within a process plant that are important for turbulence production in an explosion will be this size or smaller.

Fitting the grid around these objects would clearly require an even larger number of grid cells. This has resulted in the development of various techniques, in particular the Porosity / Distributed Resistance (PDR) approach, to allow some form of geometric representation for

large-scale scenarios, but there are uncertainties in the PDR approach as to how drag induced by the obstacles feeds into the source terms in the turbulence transport equations. However, smaller domains (e.g. flame proof enclosures) can be fully grid-resolved using current computers.

There are also the effects of the grid size on the flow calculation to be considered. Numerical studies have shown that, if the eddy break-up description is used to represent the turbulent reaction rate, then for the flame speed to be grid independent the reaction zone must be resolved by at least four cells, Catlin and Lindstedt (1991). The turbulent reaction zone thickness is around the same size as the turbulence integral length scale, which amongst obstacles may be taken as being equal to a characteristic obstacle dimension. Thus the obstacles would have to be few and large in relation to the overall geometry for the eddy break-up model to be a fundamentally sound practical approach.

The transport equations are discretized using finite differences. An idealised general requirement for the solution to a given problem, generated by a CFD code, is that the solution is grid independent - i.e. that the solution no longer varies as the grid is progressively refined. This may be impractical to demonstrate rigorously. Nevertheless, a grid dependency investigation should ideally form an integral part of CFD studies, certainly at the validation stage. The problem of obtaining a grid independent burning velocity, using the eddy break-up combustion model, is only one of the problems that may occur due to a lack of grid resolution. For example, lack of grid resolution around grid resolved obstacles could smooth the velocity profile in the shear layer caused by these obstacles, reducing the predicted turbulence generation - lowering the predicted flame speed and hence lowering the predicted explosion over-pressure. The simple CFD models do not allow grid independent solutions to be found, as these codes are generally calibrated for a fixed cell size (which is usually very large).

All of the CFD models presented in this report, without exception, model turbulent transport processes by applying the gradient transport assumption and using the two-equation, k-turbulence model to generate an effective turbulent viscosity. However, this model was developed over twenty-five years ago and not surprisingly there are several deficiencies associated with this turbulence model. First, it is important to remember that this is only a model of turbulent transport, one that has been validated / calibrated against only a limited number of fundamental flow types - e.g. planar shear layer, axisymmetric jet, etc. The model constants used for prediction of the turbulent mixing in a planar shear layer are actually different to those needed for an axisymmetric jet. Such a model is not expected, therefore, to accurately represent the turbulent processes in an arbitrary three dimensional geometry. Also, this turbulence model was developed for non-reacting, constant density flows. Hence, there is the basic question of whether or not such a model may be applied to a combusting flow without modification. Evidence suggests - Libby and Bray (1980) - that the conventional gradient transport expression (equations A13 and A14, appendix A) may not even correctly predict the sign of the turbulent flux in premixed flames - i.e. that there may be counter-gradient diffusion. Lindstedt *et al.* (1997) have conducted a numerical modelling study of flame propagation in a simple geometry (a long rectangular section tube containing a

single flat plate obstacle, aligned perpendicularly to the flow) using the k- turbulence model and a form of the eddy break-up combustion model. Lindstedt *et al.* (1997) find that although the large-scale features of the flow are well predicted, such as the over-pressure and mean

flow velocities, the turbulence intensities are not at all well predicted. Such good agreement for the macroscopic parameters may then be merely fortuitous, but further work is needed.

The eddy break-up combustion model, used by some of the 'simple' and 'advanced' CFD codes, requires a high grid resolution to yield a grid independent value of the burning velocity. The model also requires corrections to prevent unphysical behaviour near to surfaces and also at the flame leading edge to prevent numerical detonation. This has led most CFD explosion model developers to use empirical correlations for the flame speed which are grid independent and implicitly include strain rate effects. Implementation of detailed chemical kinetics through the use of a PDF transport equation holds great promise for the future, but due to the heavy demand on computer resources in terms of both processor speed and computer memory, it is unlikely that this approach will be feasible for calculations of real complex geometries for perhaps another ten or more years. Furthermore, there are large uncertainties with regards to rate data for many combustion related reactions; the combustion chemistry is extremely complex and may involve many tens of reactants and intermediate species in over one hundred reactions. It is possible to reduce the detailed kinetics schemes to a smaller number of species (maybe only five or six species), but the resulting set of species conservation equations can become mathematically stiff, with the associated sensitivity to small changes in the dependent variables. Generally, explosion models represent the combustion reactions by a single reaction step involving fuel and oxidant species only. This simplification is necessary due to present constraints in terms of both computer memory and computer speed (cf. appendix A3.2).

The models investigated fall naturally into four basic categories, empirical models, phenomenological models, Computational Fluid Dynamics (CFD) models, and 'advanced' CFD models. The differences between the three groups lie in the simplifications introduced to ease the problem solution. The phenomenological model types compromise geometric accuracy, by approximating a given geometry with an idealised model geometry, but do include reasonably advanced models for the underlying physics. The simple CFD models rely heavily on sub-grid models, such as the Porosity / Distributed Resistance model, to represent objects and, in some cases, the reaction zone. The 'advanced' CFD models allow a more realistic representation of the modelled geometry, through the use of body-fitted or unstructured grids. Grid efficiency for these latter models may be further enhanced by the use of adaptive grids, where a high grid resolution is generated only in those regions that require it. This feature also allows the reaction zone to be fully grid resolved, even for large-scale scenarios.

5. REFERENCES

5.1. Aloha TEC Documentation 2013.

5.2 Consequence analysis of an explosion by simple models: Texas refinery gasoline explosion case - aFaculty of Chemistry, Department of Chemical Engineering, University of Castilla- La Mancha. Campus 2009.

5.3 A Review of the State-of-the-Art in Gas Explosion Modelling – Health & Safety laboratory 2002.

5.4 Fire Dynamics Tools (FDTs) Quantitative Fire Hazard Analysis Methods for the U.S. Nuclear Regulatory Commission Fire Protection Inspection Program 2013.

5.5 AHE Guidelines for chemical process quantitative risk analysis 2nd ed.

5.6 Estimation of Blast over Pressures of Possible Explosion in a Furnace in Khartoum Refinery by Using MATLAB - Journal of Applied and Industrial Sciences, 2014