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Final Project Report

Title: DETERMINE THE FEASIBILITY OF TECHNIQUES FOR SIMULATING COAL DUST EXPLOSIONS

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Abstract & Keywords

The primary objective of this work is to assess the feasibility of reliably simulating the coal dust explosion processes taking place in the Kloppersbos tunnel with a computer model. Secondary objectives are to investigate the viability of simulating methane explosion suppression techniques, developing methods for minimizing the dangers of coal dust explosions, and implementing these simulations in complex mining geometries.

Existing and current work on the subject has been surveyed. A number of research groups were identified that have separately simulated aspects of the problem, including gas explosion, steady-state coal dust combustion, and detonation.

It was determined that simulations directly addressing the problem have not been performed elsewhere, but that methane explosions have been reliably modelled, and that therefore the risk would be mainly in the incorporation of dust effects. It is believed that this development is feasible, and an approach minimising the risk is suggested based on incremental development of existing programs, and validation.

Arising from the study, development is recommended in three separate areas:

1. an analytical approach,
2. a one-dimensional simulation, and
3. a three-dimensional simulation.

Coal dust explosion; computer; simulation; CFD; computational fluid dynamics; numerical; combustion model; methane; coal mine; mine safety.

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Contents List

List of Tables

1 EXECUTIVE SUMMARY

1.1 Objectives

Most experimental work on coal dust explosions in South Africa is carried out at the Kloppersbos tunnel. The primary objective of the present work is to assess the feasibility of reliably simulating the coal dust explosion processes taking place in the tunnel with a computer model.

Secondary objectives are to investigate the viability of simulating methane explosion suppression techniques, developing methods for minimizing the dangers of coal dust explosions, and implementing these simulations in complex mining geometries.

1.2 Survey

Existing and current work on the subject has been surveyed. It was determined that no suitable computer program exists which could address this problem directly. The simulation task was therefore broken up into components, and current developments in these fields assessed.

A number of research groups were identified that have separately simulated aspects of the problem, including gas explosion, steady-state coal dust combustion and detonation. Indications are that joint collaborations with some of these groups, with access to their existing programs, may enable development.

1.3 Recommendations

Arising from the study, development is recommended in three separate areas:

1. an analytical approach,
2. a one-dimensional simulation, and
3. a three-dimensional simulation.

Similar problems have been modelled in the first two areas in the past, the probability of success is high, and the resources required relatively small. However, the realism of the results will be relatively low, due to the extensive approximations that have been made.

The analytical approach can be used to perform best and worst case scenario identification. The software involved is commercial and relatively user-friendly.

The one-dimensional approach, which should be undertaken concurrently, is the first step toward simulating the process of a coal dust explosion. It has been used by other researchers to simulate gallery explosions with limited success. The program under consideration was developed by the US Bureau of Mines and the University of Michigan. It is certain that a one-dimensional analysis will not be able to simulate all the substantial processes occurring in the tunnel, and would therefore not be able to meet the project objectives by itself. However, it is a vital step towards the state-of-the-art technique, the multidimensional analysis.

A coal dust explosion occurring in the Kloppersbos tunnel or a mine is inherently a three-dimensional phenomenon. Three-dimensional simulations are complex, and computationally demanding. In view of the long development and validation times for these programs, it is recommended that an existing gas explosion program be used as a basis for development, either through purchase, or through a collaborative agreement.

A number of suitable alternatives have been identified. Those most likely are:

- Teltek in Norway, using a program named EXSIM,
- the Workcover Authority of New South Wales and the University of Wollongong in Australia, and
- the TNO Prins Maurits Laboratory in the Netherlands, using a program named REAGAS.

The choice will require some negotiation, and depend on cost, reliability and future development capability.

Since the gas industry has demonstrated the ability to model methane explosions around complex structures such as off-shore oil rigs, the risk of development is mainly in the addition of coal dust to the model. For conclusions drawn from a computer model to be built on a sound base, results from the program must be compared with experimental tests during development. Colleagues stressed the importance of the validation process and the Kloppersbos gallery will play an important role in this regard.

A detailed development plan is presented in the final section of the report.

2 INTRODUCTION

Mining coal gives rise to methane and coal dust which have caused very severe accidents. If the methane level rises above a flammable limit an ignition will cause the methane to burn. If the extent of the methane is small a flame will result, but if the methane has filled a large region the flame could give rise to an explosion. A methane explosion on its own can have devastating effects, resulting in damage to equipment and even death. In a coal mine, coal dust is present from the process of coal extraction. The methane flame moves along the tunnels and a pressure wave ahead of the flame lifts the dust from the walls, floor and roof of the tunnel. This pressure wave can pre-heat the coal dust and it burns due to the volatiles present in the coal. This process could accelerate due to energy addition from the burning fuel. A number of factors such as turbulence, obstacles, and increased pressure wave magnitude can cause enhanced burning and hence further flame acceleration. The phenomena can change from a slow deflagration, to a fast deflagration, and finally to a detonation. As this process moves towards a detonation the effects of the explosion becomes worse.

A number of experimental mines have been used in various countries to help develop understanding of the methane and coal dust explosion problem. Experimental mines are expensive to operate and therefore experimental galleries, similar to Kloppersbos, have been used to perform similar tests. The types of tests usually performed in these facilities are to determine the explosibility of various coals, the minimum initiation energy level, the level of inhibitor needed, and the effectiveness of barriers. These results are applied in the mining industry by specifying safe operating procedures or regulations. To extend the experimental results to a mining situation necessitates an extrapolation of effects. It appears that extrapolating experimental mine and gallery results to the European and American mines has been successful. They have developed safe mining operations in most cases and are scaling down their experimental investigations, Cashdollar (1994), Lunn (1994) and Margenburg (1994).

In the South African context, the Kloppersbos facility is of a realistic scale but it has a round cross-section. It seems that a fair degree of difficulty has been experienced extrapolating the Kloppersbos results to the wide range of mining techniques employed in South Africa, especially the room and pillar mines. One of the reasons for this seems to be the very different geometries in both cases. This effect could be determined by performing experiments in more realistic geometries, but this would be exorbitantly expensive due to the wide range of large scale geometries that would have to be considered.

This work addresses the feasibility of developing techniques which reliably simulate coal dust explosions in the Kloppersbos Tunnel Facility. Once these techniques have been validated they must be able to reduce the number of tunnel tests and therefore reduce the considerable experimental costs. Additional outputs from this simulation are the development of methane explosion suppression techniques, the development of improved methods for minimizing the dangers of coal dust explosions, and the implementation of these simulations in complex mining geometries.

2.1 Primary objectives

At present, most experimental work on coal dust explosions takes place at the Kloppersbos facility. In particular, gas and dust explosions are studied with the aid of the 200 m tunnel. The primary objectives of the present study are to assess:

- the feasibility of reliably simulating the processes taking place in the tunnel,
- whether simulations can replace the facility or to what extent the simulations can be used to minimise experimentation, and
- what resources would be required to set up and run suitable simulations.

The typical range of experiments, and variables involved, are described in section 3.1. The tests which are carried out in the tunnel will determine the range of situations that must be simulated. The extent that numerical simulations can replace experiments will be determined by the range that can be predicted with a suitable level of accuracy. The method selected to simulate coal dust explosions in the Kloppersbos tunnel will to a large extent determine the resources that will be necessary for this development and also the resulting accuracy of the predictions.

2.2 Secondary objectives

The secondary objectives of this study are to assess:

- whether a simulation facility could be used to develop methane explosion suppression techniques,
- whether a simulation facility could be used to minimise the dangers of coal dust explosions, and
- whether the simulation techniques can be extended to complex mining geometries.

Computer programs in this league are major pieces of software, and have useful lifetimes of the order of twenty years or more. A great deal of redesign and reworking can be avoided if the initial requirements are drawn up with a good estimate of what the code may ultimately be required to do.

The investigation therefore endeavoured to assess to some extent:

- how computer simulation may be able to contribute to improving mine safety,
- what the most likely requirements in modelling configurations other than the Kloppersbos tunnel may be, and
- how suitable flexibility could be built in at an early stage.

2.3 Investigation approach

The investigation described in this report has a number of objectives, see sections 2.1 and 2.2. To achieve these goals the following activities were undertaken:

1. ascertain whether a computer program which can be used to address this problem exists,
2. identify the most successful models of coal dust explosions and methane explosions,
3. identify South African groups engaged in related work,
4. identify the groups in the world working on the problem,
5. build a base of literature for the project,
6. understand the components involved in explosion simulations:
    - what components are essential (e.g.: capturing flame acceleration accurately),
    - what specific models are required (e.g.: modelling turbulence in a reactive multiphase flow),
    - what phenomena are well understood (e.g. shock capturing), and
    - what phenomena are not well understood (e.g. combustion models).

While the survey was carried out, it was opportune to make contact with useful groups, and

1. investigate the possibilities of collaboration where appropriate, and
2. find commercial codes and estimate their applicability and cost.

The obvious starting point for the survey was the extensive literature database maintained at Kloppersbos, and with the kind assistance of the staff a nucleus of references was located. The growing collection of relevant papers is listed in the bibliography, see Appendix A.

During the course of the literature survey, a list of the major phenomena present in the dust explosion process, and the techniques employed to model them, was accumulated and appears in Appendix F. The purpose of this collection is twofold: to identify the physical phenomena involved in coal dust explosions, and to provide a guide to the literature on a particular topic. A brief discussion of the components necessary for a simulation of these phenomena is given in section 4.1.

The active researchers in the field were identified through their publications and the recommendations of colleagues in South Africa. Names, and where available, contact information, are listed in Appendix C.

A number of computer programs emerge as known achievers to date, or having elements relevant to this project. Some of their properties and the techniques used are summarised for comparative purposes in Appendix E. A discussion of those immediately relevant and work that may prove useful to the project is summarised in section 4.2.

It should be noted that the survey concentrated on numerical modelling of dust and gas explosions. There is an enormous amount of underlying literature on many aspects important to understanding the process, and where appropriate for future reference, publications of related interest have been included in the list, see Appendix A. The reader will therefore not find an exhaustive survey of dust particle combustion or non-combusting shock waves in dusty gases. There are, however, a number of papers which may serve as entry points to the literature of the related fields of, for example, pulverised coal boiler modelling, combustion modelling, and explosibility measurements.

3 NEEDS OF LOCAL INDUSTRY

The immediate task of this project is to assess the feasibility of simulating the Kloppersbos tunnel. A survey of the types of experiments carried out in the tunnel is given here, and were used in identifying variables and configurations which affect the choice of simulation technique, see section 3.1.

Engineering software of this type would be expected to have a useful lifetime of decades, if the fundamental design is sufficiently flexible. In drawing up preliminary functional requirements for the simulation program, there are advantages in having an understanding of the secondary objectives of the project. We have therefore attempted to form an idea of the alternative uses to which coal dust explosion simulations may be put to improve mine safety, and, in particular, the configurations which would be required. If development is successful and the short-term objective is achieved, i.e. to model the tunnel, but has no development path to the final objectives, i.e. to improve safety in coal mines, the result would be a waste of scarce development resources. Two future applications have been identified: local explosion simulation and global explosion propagation simulation, see sections 3.2 and 3.3.

3.1 Kloppersbos 200 m Tunnel Simulation

If a simulation is to replace experimental tests, the simulation will have to predict the physical phenomena with a suitable degree of confidence. The accuracy of the simulation will usually be determined by comparing predicted to measured parameters such as pressure, flame position and temperature. The numerical simulation will have to predict at least the data which is being measured in the tunnel and hopefully more data will be generated. The experiments carried out at the Kloppersbos tunnel fall into three major categories, these being concerned with:

- explosion hazards,
- preventative measures, and
- protective measures.

Comparative tests are carried out with or without various preventative or protective measures; the final results are frequently in the form of "go" or "no go", indicating whether an explosion is effectively suppressed or not.

In table 1 the various experimental phenomena are listed in the form of a set of components that need to be simulated. The requirements are not all equally important; for example, modelling of vents has a very low priority, while adequate modelling of combustion will be crucial.

Table 1 contains the translation from the experimental conditions to the capabilities that would be required by a computer simulation. However, the descriptions do not yet determine the type of model or mechanism to be used. For example, a dust lifting model of some sort is required; a very simple mechanism would be to assume that the dust is initially homogeneously distributed throughout the tunnel volume, while a sophisticated lifting model could be envisaged which simulate a layered dust problem. This would mean that the model would have to describe the mechanisms by which particles are lifted into the flow. The table also presents a perceived importance associated with each phenomenon. The importance of each component will determine the level of approximation that can be used for that component in the simulation.

Table 1: Kloppersbos experimental phenomena and simulation requirements

Physical phenomenon	Simulation requirement	Priority
Fluid flow		
pressure wave	inviscid fluid model	high
blast wave/shock wave	shock capturing or shock tracking.	high
Explosion hazards		
methane 5-15% in first 7 m of tunnel	two-phase model or equivalent	high
deflagration wave (methane only)	methane combustion model and turbulence model	high
coal dust combustion, deflagration with dust	dust lifting model	high
	dust devolatilization model	high
	coal volatiles combustion model	high
	interaction of turbulence with particles	medium
	interaction of particles with turbulence	low
detonation wave	deflagration-to-detonation transition (DDT) model	low
	capturing of detonation wave	low
Preventative measures		
stone dust/inert dusts	inert dust effect on extinction	high
	interaction of turbulence with particles	medium
	interaction of particles with turbulence	low
binders	decreased dispersability	medium

Table 1: continued

Physical phenomenon	Simulation requirement	Priority
Protective measures		
passive measures	vary location of suppressant source	medium
	trigger source by detecting pressure wave	medium
active measures (powder, gas or water)	vary location of suppressant source	medium
	other trigger mechanisms, e.g. flame in line of sight	medium
	extinguisher models (powder or gas)	low
explosion-proof stoppings; walls	obstacles in flow	medium
Internal geometry of tunnel		
gallery configuration	simple grid	high
walls, closed end	reflecting boundary conditions	high
open end	external boundary conditions	high
diaphragm	initial conditions for species concentration, pressure	high
diaphragm bursting	point of rupture model	medium
dust shelves	obstacles in flow	medium
side doors/vents	external boundary conditions	low
Ignition source		
point source	small spherical initial flame	high
volumetric source	initial propagating plane flame front	high

3.2 Mine Geometry: Small Scale Studies

According to the recent SIMRAC report on safety-related needs of the coal mining industry, see Phillips and Landman (1994), of the order of 66% of explosions and ignitions occurred in the region of the face (for incidents of known cause during 1989-1993). The major ignition source is frictional, particularly cutting picks on continuous miners, coal cutters and shearers. Flames from blasting, heated surfaces and spontaneous combustion, and electric sources, account for smaller percentages. Internationally, these explosion sources have been controlled using special cutting picks, inhibitors and triggered barriers. Flame proof enclosures and an "ultimate" triggered barrier are still being investigated in Europe, Margenburg (1994) and Lunn (1994).

Should it be desirable to model the initial development of explosions at these sources, and the effectiveness of suppression measures located near the sources, the simulation requirements are slightly different from those for the Kloppersbos tunnel. The major difference is more complex geometry, particularly because the presence of continuous miners, conveyors or cars in the roadway will influence turbulence and flame speeds very considerably. Grid generation and configuration would therefore be more demanding; multidimensional models are essential; the number of cells required to resolve features of interest will be large; and good representation of obstacles may require a body-fitted grid.

Under these conditions, DDT and detonation should not be encountered, but the ignition, initiation phase and development of the flame (laminar and turbulent) will be important. This requirement may be less critical for the tunnel, since it can be initiated at a later stage in the explosion process and usually the flame is turbulent well before the phase of interest, i.e. when measurements are made.

If reasonable suppressant models become available, simulations on this scale could be used to estimate the effectiveness of different systems; for example, extinguishing systems located on continuous miners.

To the authors' knowledge, no work of this kind on dust explosions has been carried out anywhere. The simulations most closely related would be those of gas explosions in clouds released from chemical process plants with complex vessels, buildings, or on off-shore platforms, see publications by Hjertager, van den Berg and van Wingerden.

3.3 Mine Geometry: Global Propagation

The modelling of substantial areas of a mine in which explosive fronts are propagating poses complex geometrical requirements. It has been found, in gas explosion simulations, that it is important to simulate the initial development of the explosion because the initial process has a large influence on the resultant explosion. Therefore laminar development and ignition properties should be modelled, either as an integral part of the global propagation or as a separate solution which is used as input to the global simulation. In addition to the geometry of the headers, roadways, etc., the effect of cars, mining machines and other obstructions must be captured; since good resolution increases the number of cells and hence the run size and time, a compromise is always reached between resolution (simulation accuracy) and the size of the grid (run times).

In addition, ventilation properties are required as boundary conditions. The propagation of fast fronts must be well simulated, while DDT and detonation are possible but improbable. Preventative or protective measures may be present and so extinction should be well modelled. In this configuration and the local studies, section 3.2, the initial concentration of methane and coal dust is critical to the overall result and must be determined. When comparing to an experimental mine result the experimental set up will be clearly defined, but for a mine simulation this information will be hard to obtain. The methane and coal dust levels will have to be determined by linking ventilation and diffusion simulations. The ignition source can then be used to start the simulation from the initial concentration distribution.

Simulation runs are likely to be relatively long for this type of simulation, and experimental data for validation will hard to obtain, other than those measured at Dortmund EM, see Michelis *et al.* (1987). With reasonable confidence in the code and good computing resources, it should be possible to optimise the siting of inhibitors, extinguisher or protective systems; study the effect of mine layout on explosion propagation; and conduct retrospective studies after accidents.

Portions of a mine have been simulated with a two-dimensional approximation (a plan view), see Green *et al.* (1991), using a model in which only the methane explosion was considered.

Gas explosion codes, being more mature than those including dust, have been applied to extended complex geometries such as off-shore platforms, see publications by Hjertager, van den Berg and van Wingerden. Validation of these results has to some extent been achieved by comparison with scale models. These codes suffer from the insurmountable problem that they have to model physical obstructions far smaller than their grid resolution capability and therefore the problem scale is critical. In the coal dust explosion case the problem of scale is also critical because of its influence on explosion parameters, see Moen (1993). When validation is carried out it will be critical that geometric scaling is kept in mind, to benefit from the experience of the gas explosion industry.

4 SURVEY OF EXISTING WORK

4.1 The Components of a Simulation

Before evaluating the existing work relating to coal dust explosions, a brief description of the computer simulations considered here is in order.

A computer model comprises a number of component models, each of which attempts to mimic a particular phenomenon. The choices for component models may include an analytical formulation, a data-base approach, an empirical formulation or a numerical approach. The numerical model usually entails solving a set of ordinary or partial differential equations on the points of a grid filling the zone of interest. It may be noted that the term "sub-model" in this field usually refers to the simulation of effects on scales smaller than the grid spacing, i.e. those not resolved by the grid.

A brief description of the necessary components of a simulation for reacting flow incorporating dust is given in Appendix D. The major parts are listed here:

- fluid flow model
- solver
- chemistry
- turbulence model
- combustion model
- inert and coal dusts, e.g. lifting models
- dust devolatilization and volatile combustion
- models for other substances, e.g. water
- obstacles and geometric effects
- boundary conditions
- radiation.

Appendix D also contains a brief discussion of the importance of validation in developing a simulation whose results are useful.

4.2 The Most Relevant Models

As was mentioned above, no model was identified which could be used to address the objectives of this project without modification and development. A number of related models were identified, and brief descriptions of them are given in this section.

4.2.1 South African developments

It is of interest to note that Bonapace (1990) developed a one-dimensional analytical model of the Kloppersbos tunnel, based on a pressure wave description, which could be analysed in terms of the telegraph equation. The effects of turbulence and combustion, etc., were included only through constants which were obtained by experiment, and the analytical solutions of the tunnel equation compared qualitatively with tests. The absolute values of pressure were under-predicted by approximately 100%. This method, being based on tunnel specific constants, has limited scope for further application.

The present quest for numerical methods may be seen as a logical consequence of this work in the development of a predictive tool.

A number of South African universities have developed their own Navier-Stokes CFD programs using the SIMPLE algorithm (similar to PHOENICS) e.g. the University of Pretoria and Potchefstroom. These are development programs which means that a number of authors have been involved, validation is usually uncoordinated and their capabilities are limited. If the more applicable gas explosion codes can't be obtained due to collaboration problems or excessive cost then the this avenue of development will be investigated. This will mean further CFD development of the university programs and extensive validation.

4.2.2 Software written in association with the coal mining industry

Some investigation into numerical modelling of coal dust explosions has been carried out at the United States Bureau of Mines. A model of a coal dust explosion propagating along a mine roadway was performed by Davies (1974), who modelled a thin flame separating the burnt and unburnt gases using a simple laminar burning velocity law. Edwards *et al.* (1977), Edwards and Ford (1988) and Edwards (1990) developed a number of mathematical models for the spreading of fires and coal dust explosions. Their models were based on the important work of Jones (1958) and Pickles (1982) who considered laminar and turbulent flames. Source terms were included for coal dust and rock dust. Chi and Perlee (1974) produced a one-dimensional program which was later developed, see C O Lee (1991), to include layered dust explosions, a sub-model of dust dispersion, and a turbulent combustion sub-model. Some results are presented by Chang *et al.* (1987) and Sichel *et al.* (1994). This appears to be the most advanced one-dimensional code in use today, and it is likely that the source code is in the public domain.

A one-dimensional and partial two-dimensional simulation of the Dortmund Experimental Mine in Germany was performed by Esser, see Grönig (1994). A gas dynamic code using a Riemann solver was linked to a combustion model using the experimentally measured flame position as input to the simulation. Aachen University is in the process of developing methane combustion models using a flame tracking approach but this work is still in the development phase, see Kirmess (1994).

Green *et al.* (1985) (1993) developed a viscous three-dimensional model using a TVD approach. Turbulence is modelled using the $k-\varepsilon$ model and combustion uses a one-step eddy breakup model. This program can only simulate the combustion of methane and the inclusion of dust is under development, see Green *et al.* (1993). Some validation was performed using experimental data from the 10 m Norfuss ignition tube which has 5 annular baffles; excellent agreement was obtained for pressure and reasonable agreement for peak velocities. The simulation was also found to capture acoustic modes (which have been shown to affect flame velocity). This program was then used to simulate the explosion that occurred in the Moura Mine in 1986. A two-dimensional (plan view) methane model of two cross-cuts and two headings was created. The model included the presence of a continuous miner, shuttle cars and a diesel rover. Comparison between the simulation and forensic evidence was used to validate the model partially. The main drawback with this program is that it runs on a transputer system which is not a standard system and development is under way to move this program to a work station, Green (1994).

Very interesting simulation work was begun in Britain at the Health and Safety Executive, in association with the Buxton Experimental Mine (Lea (1993)). Three computer models were run in conjunction with one another:

- the US Bureau of Mines network code (MFIRE) was used to provide one-dimensional boundary input values,
- a gravity current model developed by consultants predicted the growth and breakdown of currents in the presence of a background flow, and
- a three-dimensional computational fluid dynamics code FLOW3D, from Harwell, was used to model the local region of the fire.

Published results for a possible diesel fire were promising. The group is pursuing the computational approach for fires and have started to consider fireproof enclosures which will involve explosion simulations. All the numerical development is being performed within the code FLOW3D.

Some simulation work takes place in Poland, in association with the Barbara Experimental Mine. The present authors have had difficulty in obtaining published literature, but are in the process of establishing the details of this work, which seems to have been performed by Wolanski, see Lebecki (1994) and Sichel (1994).

INERIS, in France, have developed a computer program for simulating the local effect of triggered barriers in headings, Proust (1993). Propagation and extinction is modelled in a methane/air/water-droplet mixture. The details of this models were unknown at the time of publication of this report.

4.2.3 Software developed by the gas industry

There has been considerable investment by the companies with an interest in North Sea gas in modelling hydrocarbon explosions, in attempts to improve the safety of off-shore oil platforms. A number of universities and institutes have developed simulation programs, and some of these currently represent the state of the art in gas explosion modelling, being considerably more mature than those sponsored by other industries. Several are in the process of commercialisation.

These programs have recently found extensive application in other areas, notably modelling of explosions in process plants.

Our team was fortunate in being given access to the results of a Commission of European Communities programme (MERGE) to compare the performance of the major gas simulations (Arntzen *et al.*, 1994). In this study, five computer programmes were compared, beginning with tests at small and medium scale in which the teams were allowed to adjust parameters to improve results, and a third blind test at large scale in which predictions were compared with experiment. The test configurations were methane or propane explosions in a cubic volume penetrated by pipes of different diameters and separations.

One of the most important aspects of these codes is their reliance on sub-models, into which a great deal of development effort is currently being invested. The sub-models are responsible for grid-dependent results, and are critical in determining the behaviour of the flame model, turbulence, turbulent combustion, and drag.

The details of the MERGE comparison is provided in Appendix E. In summary, reactive CFD has progressed dramatically in the field of gas explosions due to the high level of funding and the wide interest in the field. The cost of developing simulation software in this league took approximately 10 years and 20 man years. The numerical developments were linked to extensive experimental studies and this increased the development cost substantially. These gas explosion codes have reached a relatively mature level of development. The are used by designers of off-shore rigs, as input to codes of practice and regulations, and in accident investigations. These programs have a large proportion of the basics required for an advanced coal explosion simulation program. The main components as described in section 4.1 which they lack are:

- coal dust chemistry,
- inert and coal dusts, e.g. lifting models,
- dust devolatilization and volatile combustion, and
- radiation.

Some components of the simulation may require modification such as the turbulence and combustion models. It therefore seems logical that if a coal dust explosion program can be based on an advanced gas explosion program then substantial savings can be realised. Estimates made by various researchers in the gas industry of the effort necessary to perform this extension were two to three years and one to two man years per year. This effort would result in a program which could simulate the dominant effects making use of the necessary simplifications. The gas explosion industry were unanimous in their belief that the coal dust explosion problem was difficult to model, but that with the necessary resources it could, however, be simulated. Various groups were also starting to develop models in the dust explosion area but with the emphasis on industrial dust explosions.

There is a considerable amount of further work appearing in the literature on gas explosions, which may be found in the bibliography. The notes in Appendix E cover the software of interest to this project.

4.2.4 Commercially available general purpose software

A number of general purpose CFD packages are commercially available and use similar methods to those used by the gas explosion industry. Some examples of these are PHOENICS, STAR-CD, FLOW3D and CONCHAS-SPRAY. Aerotek has used PHOENICS for a number of years and is evaluating STAR-CD at present as an alternative to PHOENICS. None of these programs can solve a coal dust explosion problem in its present form. FLOW3D is being developed to include combustion models similar to those used by the gas explosion programs, Lea (1994). Kjäldman (1992) has used PHOENICS to model slow deflagrations in a standard spherical test vessel. No direct comparisons were made with experimental values and the model was said to be relatively crude. STAR-CD has not yet been applied to this problem but makes use of the PISO algorithm for unsteady simulations, which has been demonstrated to be superior to than the SIMPLE algorithm which the other programs use.

The addition of the various dust models will necessitate extensive additional program development. These programs are generally available in non-source form, which means that modification or addition to the program has to be done via complex, external user defined module addition or through development agreements with the suppliers. It will be difficult for these programs to form the necessary development platform and are therefore not a viable option. The only exception is FLOW3D, for which the source code is available and developments in this area are presently under way through the UK Health and Safety Executive.

4.2.5 Software developed by other industries/universities

A number of computer programs have been developed by industries not directly related to the coal mining or gas industries, but which are nevertheless of interest to this investigation. The first group of programs address the gas dynamic, thermodynamic and chemistry problem. The programs developed by various institutions are: TIGER, NASA and STANJAN. Combustion Dynamics Ltd. have combined the features of these programs into a user-friendly program called SuperSTATE, which runs on a PC, see CD Ltd. brochures. The user specifies an initial state and a process, and SuperSTATE calculates the conditions subsequent to the process. SuperSTATE costs US$ 4.5 k for a single user licence with no source code. This type of program can be very useful for initial order of magnitude analysis. SuperSTATE is incapable of modelling the actual coal dust explosion process, but it could be used to construct and analyse a series of steps which approximate the process. Computational resources used for this program are insignificant and therefore some parametric evaluation of the process can be performed. Other processes like flames could be added by CD Ltd.

Oran and Boris (1987) and colleagues have produced a family of programs based on FCT numerical methods and a variety of chemical models, including the two-step induction parameter model. An early development was the program SHASTA, by Boris and Book (1973). These programs appear to capture discontinuities well, and have been used to simulate phenomena like muzzle blast, planar mixing models, combustors, and propagating detonations including detailed cell structure. The group has also written separate Lagrangian models for droplet behaviour in shear flow. Possibilities for collaboration have not yet been investigated.

Integrated Fluid-Structure Analysis Software (IFSAS) contains a CFD simulation capability, see CD Ltd. brochures. This program solves the Euler equations using the FCT approach (similar to Oran and Boris), it is time accurate, three-dimensional and uses a Cartesian grid. It includes combustion, with a one-step and two-step combustion model (Thibault, (1994)). This program operates in a user-friendly environment and presently costs US$ 25 k for a single station with no source licence. IFSAS is based on inviscid flow and CD is currently developing a Navier-Stokes program, SuperCFD, which will put them in the same league as REAGAS, EXSIM and FLACS. The main draw-back with this development is that it is not in FORTRAN but in C++, which impedes collaboration with other groups. Collaboration could still be possible but the details of which would have to be discussed via MREL.

The most sophisticated computer models of the microscopic processes occurring in the combustion of coal particles appear in simulations of coal-fired boilers. This field has the advantage that more detailed particle models may be incorporated because computer time is shortened by the requirement for steady state solutions only: time dependence is not important.

Comprehensive combustion models are reviewed by Hill and Smoot (1993), who are also the authors of the successful program PCGC-3 designed for pulverised coal boilers. The three-dimensional Navier-Stokes equations are solved with a modified SIMPLE method, $k-\varepsilon$ turbulence, full equilibrium chemistry, radiation, and NO_x formation. Detailed Lagrangian particle tracking allows devolatilization, particle swelling, and particle influence on turbulence to be modelled - all phenomena which the coal dust explosion field could incorporate, when time permits. Depending on the modularity of the PCGC programs, it may eventually prove possible to make use of selected material from this field.

A very active group working on vapour cloud explosions and gas detonations is based at McGill University. This group has experimentally established a detailed knowledge of the mechanisms of explosion, detonation, and DDT (Moen *et al.* (1982, 1983, 1986, 1993), Shepherd *et al.* (1986), Lee and Moen (1980), Lee *et al.* (1982)). In particular, cell structure, induction time, geometric influences, auto-ignition, SWACER, and acoustic mode/flame front coupling have been covered by this group. Numerical simulations have been carried out with the aid of FLACS, see Moen *et al.* (1986).

5 SIMULATION OPTIONS TO MEET OBJECTIVES

No software was found that could satisfy the objective of this project directly. This led to the analysis of the industry needs and a survey of existing work. The primary objective, to model the Kloppersbos tunnel, is a short-term objective and the secondary objectives address the long-term goals of the project. To achieve both the primary objective and the secondary objectives it is necessary to consider the general simulation requirements of coal dust explosions. The simulation requirements can be divided into three geometric levels:

- Kloppersbos tunnel or gallery,
- local mine area, and
- global mine layout.

The simulation can also be divided into three broad processes:

- methane explosions (initiation and propagation),
- coal dust explosions (propagation), and
- termination phase: inhibitors/suppressors/barriers.

Each of these processes can occur in any of the above geometries. The simulation complexity can be divided into a few broad categories with an associated computational resource requirement.

• experimental data processing and extrapolation,	PC to WS
• analytical simulation,	PC to WS
• one-dimensional analysis with empirical correlations, and	PC to WS
• multidimensional analysis with empirical models.	WS to SC

To achieve the project's objectives, a comprehensive and well-balanced capability is required. It is proposed that the full range of approaches enumerated above should be considered.

The data-base analysis approach would rely on the experimental results of the Kloppersbos tunnel and any other data which could be obtained. Any simulation results from this approach would therefore be limited to experiments that have already been performed, and would have very limited extrapolation capability. To achieve either the primary or secondary objectives this approach is not considered be a viable option.

Each of the next three levels of analysis is presented below, and possible approaches for each will be described.

5.1 Analytical Approach

These developments have been described in section 4.2.5 and essentially only one viable option was identified. To summarise, the TIGER, NASA and STANJAN programs have been incorporated into a user-friendly program which runs on a PC, SuperSTATE, by Combustion Dynamics Ltd. SuperSTATE costs US$ 4.5 k for a single user licence with no source code. This type of program can be very useful for initial order of magnitude analysis. It is incapable of modelling the actual coal dust explosion process, but it could be used to analyse various processes which approximate it. Computational resources for this type of model are unsignificant and therefore some parametric evaluation of the processes can be performed. The user can get some overall estimates of over-pressure and loading quickly and easily, but the actual coal dust explosion process can't be simulated.

This software is commercially sold and therefore it should been reasonably well validated, and have inherent validity, back-up and the possibility of future development. Only a PC will be required to run this software and a solution will take seconds or at most minutes. Any user with a basic understanding of gas dynamics and thermodynamics could use this program, and limited computer knowledge would be necessary due to its user-friendly interface. One avenue which might have to be investigated would be a multi-user licence so that this program could be used by a number of different sites simultaneously.

5.2 One-dimensional Analysis linked to Empirical Correlations

Various institutions have considered this approach and these developments have been described in section 4.2.2. In these models the flow is solved using a one-dimensional CFD approach and the other effects are included by empirical models, e.g. the lifting of the dust. The program developed by Chi and Perlee (1974) and modified by C O Lee (1991) appears to be the most advanced one-dimensional code currently in use. This program is used at the University of Michigan and it seems that the source code will be free of charge. Although a one-dimensional program can't address all the dominant phenomena, it can be an extremely useful analysis tool, the reasons for this are:

- limited computational resources are necessary, i.e. only a PC,
- the program is relatively simple,

- basic phenomena can be easily evaluated,
- empirical models can be cost-effectively evaluated, and
- numerical algorithms and approximations can be evaluated at low cost.

Collaboration on this piece of software with the University of Michigan is possible, see Sichel (1994), either directly with Aerotek or with a South African University, e.g. the University of the Witwatersrand. The one-dimensional approach has shortfalls and they are as follows:

- unable to consider geometric effects,
- unable to model multidimensional effects,
- unable to model turbulence,
- input to empirical models will be limited to one-dimensional behaviour,
- it is a research program and not developed in a controlled fashion, and
- validation and development has been uncoordinated.

The authors consider this type of tool as an essential bridge between the simple analytical and complex multidimensional analysis procedures, because it addresses more complex issues than the analytical approach with limited development cost or risk.

5.3 Multidimensional Analysis linked to Empirical Models

An original local development using a similar approach, as used internationally, can be considered to require similar resources as the international developments. A simulation development of this nature has been determined to take approximately 10 years and require 20 man years (an average of various international development programmes). To develop this program extensive experimental input will also be required which has a cost similar to the numerical development. The estimated total development cost of an original South African capability is considered to be exorbitant and therefore not a viable development option.

In the multidimensional area extensive development was identified, but in most cases it was found to be in associated fields. This implies that further development will be necessary to achieve the project objectives. The proposed development strategy in this area is to use an established and validated program as a basis for further development. This is believed to be the most efficient means of developing a capability in coal dust explosion simulation, i.e. a balance of development risk, cost and duration. To select a suitable program as a basis for further development, a number of factors must be considered and these are presented in table 2.

Table 2: Available software: capabilities, cost and collaboration possibilities

Group	Program	Current capability	Cost (kR)	Collaborate	Maturity
Tel-Tek	EXSIM	Gas explosions	Joint devlp.	Easier	Moderate
CMR	FLACS	Gas explosions, dust being devlp.	2000/year	Difficult	High
TNO	REAGAS	Gas explosions	Joint devlp.	Easier	Moderate
CD/MREL	IFSAS	Explosions (inviscid)	100	Difficult	High
WANSW	Green	Gas explosions	Unknown	Moderate	Low
B-GAS	COBRA	Gas explosions	Unknown	Unknown	Unknown
UK AEA	FLOW3D	General, fires and gas explosions	80 + 30/year	Moderate	High

The Naval Research Laboratory (USA), Barbara EM (Poland) and INERIS (France) have also been identified as being involved in simulation but the details regarding their computer programs was not known at the time of publishing this report.

The estimated cost and ease with which collaboration can be achieved has been given in table 2. At this stage, no detailed collaboration discussions have been entered into. The reasons for the comments about collaboration, included in table 2, are as follows: FLACS had a high development cost covered by the gas industry and it will be costly to obtain or require complex contract negotiations; EXSIM and REAGAS should be easier as EXSIM was developed at a University and REAGAS has been used in joint developments previously (e.g. with INERIS of France); IFSAS will be difficult because of the computer language used (C++) and no source is available; Green's code is possible but this program makes use of an unusual computer system, which complicates interaction; and FLOW3D is a viable option but relatively costly because it must be purchased, but once it is purchased it can be modified as necessary.

If any one of the above computer programs is obtained either by purchase or through collaboration, a number of activities will have to be performed to achieve useful simulation results. It will have to be ported onto the particular computer system available, compilation differences removed, and the results verified by running a number of test cases. The capability to predict gas explosion propagation through complex geometries will then exist in South Africa if FLACS, EXSIM, REAGAS or Green's program is selected. IFSAS in its current form is inviscid and does not have the capability to consider viscous flows. FLOW3D may require additional modification to reach the level of capabilities of the gas explosion programs.

This program should be able to simulate methane explosions in the Kloppersbos tunnel and in a mining layout with a similar level of confidence as in the gas industry, i.e. about 50% accuracy on overpressure.

The reliability of this base CFD software will largely depend on which program is selected as each has reached a different level of maturity and validation. An indication of the perceived level of maturity of each program has been given in table 1. The level of software maturity has been ranked based on the level of commercialisation, the user interface and the level of validation. None of the information provided in table 2 should be taken as definitive or absolute, but purely as an indication of the present situation as perceived by the authors.

When this program has been used to analyse methane explosions, the next step will be to add the components necessary to simulate coal dust. This process will involve both numerical and experimental development. Numerical development will take place in the areas where the effect of the dust can simulated by mathematical models. Experimental development will be essential in areas where the physical phenomena can't be modelled at present and an empirical model will have to be linked to the numerical model. Experimental measurements will also be necessary for validation, unless suitable experimental data already exists.

After the development of the coal component of the numerical model, this program should be able to meet the objectives of the project. This means that the safety needs of the mining industry can be addressed by means of numerical simulation. This will only be true if the development program is successful, which is by no means guaranteed because it has never been achieved to date. The simulation accuracy should only be limited to the present level of numerical simulation technology and the level of approximation employed. Confidence in the simulation can only be measured and developed through validation, i.e. comparison of numerical results with experimental results.

Opinions on whether coal dust explosions can be successfully simulated are varied. The established mining industry is sceptical (USBM, UKHSE), the applied research companies (CD, MREL, CMR, TNO) believe that with sufficient funding the main features can be modelled, and the Universities believe that given sufficient effort it can be done. It is generally agreed that this problem combines all the possible complexities a numerical model could have and would be a model at the leading edge of numerical research. This confirms that it will be critical to select a development path which offers a suitable risk to investment balance. Experimental input to this process will also be essential in the realms of empirical model development and validation. A comment was also made that collaboration with international institutions might be easier to achieve via "interesting" experimental results than by numerical developments, Moen (1994).

The cost of developing a gas explosion model into a coal dust explosion simulation program is determined by the development method employed. The method that will be used is not defined at present, but if a development strategy similar to the gas industry is used, i.e. incremental improvement, an approximate cost can be determined. The gas industry estimated that if one to two people worked full time for two to three years some useful results would start to emerge. This level of effort was considered to be the minimum level that would ensure positive results. Development should be focussed at the dominant phenomena and these could be experimentally determined.

The cost of running a model of this nature will depend on the problem complexity. These models must generally be run on powerful computers: work stations or super computers. As computers continue to develop, this type of simulation may be able to be run on a PC if either the problem complexity is reduced or long run times are acceptable. Generally, a run of this nature takes between hours and days on a work station with sufficient memory (e.g. 64MB).

Maintenance of a piece of software which is under development is difficult. The level of control that is exercised over the software will depend on the end application. Software control is essential if reliability, accuracy and repeatability is necessary. A number of forms of control exist and these range from simple development guidelines and change control to full software engineering. A suitable compromise must be reached before software development proceeds.

The user of this program requires different skills from those required by the previous simulation programs, sections 5.1 and 5.2, because this program will be an advanced CFD package. It can be made accessible by having a user-friendly interface, but will still usually need a person who understands CFD. Uninitiated use of CFD can have disastrous consequences and a user must either have an good understanding of the problem being solved or the methods being used, and preferably both. The other limiting factor that determines who could use a simulation program of this nature is the computational requirements, which are large and not widely available.

6 CONCLUSIONS

The feasibility of developing techniques which reliably simulate coal dust explosions in the Kloppersbos Tunnel Facility was the primary objective of this investigation. Secondary objectives of this investigation were to determine the feasibility of simulating methane explosion suppression techniques, developing improved methods for minimizing the dangers of coal dust explosions, and implementing these simulations in complex mining geometries.

It was determined that no simulation program exists which could address the above problem and that no organisation, national or international, was considering this problem directly at present. The process of a coal dust explosion was broken up into its various components, and the current simulation development in each of these areas was investigated.

For a simulation exercise to be successful the safety needs of the South African Coal Mining Industry, available development resources, current computational resources and level of simulation must be matched. As much information as possible was gathered during this investigation in an attempt to evaluate the feasibility of achieving the necessary level of synergy.

A number of research groups were identified that had considered simulating various aspects of the problem. Some groups have modelled explosions in gas clouds and developed sophisticated CFD programs for this purpose. Other areas that were identified include detonation modelling, shock waves in a dusty gas, steady coal dust combustion, deflagration-to-detonation transition studies, fire modelling and coal dust experimental investigation.

The project goals and available technology comparative analysis led to the conclusion that this problem could be addressed at a number of different levels. Each level will require a different modelling strategy, with a certain level of approximation inherent to the method, and therefore different resources will be necessary and the confidence associated with the results will be different. It is proposed that development starts with a simple method first, and then progresses towards the more complex approaches. The main reason for this suggestion is that the cost and risk can be minimised, and then incremental development can be used to achieve the high risk goals. The ideal approach, a three-dimensional analysis, has never been successfully demonstrated and success is therefore not certain. The risk of developing a simulation program which is believed to be capable of solving all the project objectives is therefore high.

Development is recommended in three separate simulation areas:

1. Analytical approach
2. One-dimensional analysis
3. Multidimensional analysis

The first two areas have been well explored in the past, the probability of success is high and the resources required are relatively small. The realism of the results is unfortunately relatively low due to the extensive approximations that have been made, but due to their simplicity they would both be able to run on a PC.

An analytical simulation can be used to perform best and worst case scenario identification. A one-dimensional method is the first step in trying to simulate the actual process of a coal dust-explosion. This approach has been used by various researchers to simulate a gallery explosion and has yielded mixed success. It is certain that a one-dimensional analysis would not be able to simulate all the processes which occur in a tunnel, and therefore would not be able to meet the project objectives by itself. The authors, however, consider this step as a vital one towards the ultimate analysis technique, the multidimensional analysis.

An analytical method or one-dimensional analysis method will be able to model some of the phenomena which occur in the Kloppersbos tunnel, but offer limited opportunity for extension to mine layouts. A coal dust explosion which occurs in the Kloppersbos tunnel or a mine is a three-dimensional phenomenon. The only possible means of simulating this reasonably accurately would be to perform a three-dimensional analysis, which is a complex and expensive process. A powerful computer is necessary, the computer must have sufficient memory and run times are usually long. It has been determined that the best approach in this regard would be to base the three-dimensional coal dust explosion simulation development on an existing gas explosion program. A number of suitable alternatives have been identified, but the details regarding purchase or collaboration would still have to be finalised before a decision regarding which program or institution to work with can be taken. This decision will be made based on cost, reliability and future development capability.

In conjunction with the three-dimensional program an empirical development activity will be necessary. Not all phenomena can currently be modelled and these will need empirical models to describe their behaviour. Experimental results will also be crucial for the validation of the simulation results, which must be an on-going process during development. The feasibility of reliably simulating a coal dust explosion using a three-dimensional analysis is uncertain. The gas industry has demonstrated the ability to model explosions in gas clouds around complex off-shore rigs but a coal dust explosion has not been solved yet. The risk of development is therefore mainly associated with the addition of the coal dust to the model. For example, models of coal dust lifting, kinetics, devolatilization and volatile combustion, as well as combustion product development and kinetics will be required. The effect of coal dust on turbulence is also an effect which is not well understood at present. The gas industry programs also deal with numerous simple obstacles, whereas this problem will have to consider a few complex obstacles, which might necessitate a different CFD approach.

In conclusion, it is generally accepted that the reliable simulation of a coal dust explosion in the Kloppersbos tunnel is a challenging objective, even more so the extension to mine layouts and suppression analysis. The authors believe that by undertaking a well controlled and incremental development approach the major phenomena can be successfully simulated. The details of the proposed strategy have been presented in the Recommendations.

7 RECOMMENDATIONS

The proposed development plan to achieve a reliable simulation of coal dust explosions will require resources of one to two man years for 2 to 3 years before directly applicable results will be achieved (activities 1 to 7 below) and the development can continue beyond this point as described below.

1. Establish an analytical capability by purchasing (at a cost of US$ 4.5k) and using, SuperSTATE: a program developed by Combustion Dynamics Ltd of Canada. Use SuperSTATE to determine which phenomena of a Kloppersbos explosion can be simulated in this approximate manner.
2. Concurrently with 1, establish a one-dimensional analysis capability by obtaining (hopefully free of charge), studying, commissioning and applying the program as finally developed at the University of Michigan, Sichel (1994). Use this program to model the Kloppersbos tunnel, and determine its applicability, accuracy and possibility for development.
3. Develop a strategy most appropriate for establishing a three-dimensional gas explosion capability, either via purchase (cost to be determined) or collaboration (details to be negotiated) with an international institute. Cost, risk and future development capability must be assessed when selecting the institution/program.
4. Through careful experiment, identify the dominant coal dust explosion phenomena for which model components must be added to the simulations, study the available empirical models, propose and develop suitable new empirical models where necessary.
5. Carry out the process developed under (3), i.e. commission gas explosion program.
6. Implement (4) in the one- and three-dimensional analysis (where applicable). The result of this activity must be a one- and three-dimensional dust explosion analysis capability. Development in this area will be on-going, as improvements which are worth implementing are identified.
7. Validate (6) using experimental data from Kloppersbos, other galleries or experimental mine facilities.
8. Develop methane explosion suppression models and incorporate them into the simulation: ventilation, and active suppression.
9. Validate (8) using data from Kloppersbos, other galleries or experimental mine facilities.

10. Develop coal dust explosion suppression models and incorporate them into the simulation: stone dusting, barriers, stoppings and active barriers.
11. Validate (10) using data from Kloppersbos, other galleries or experimental mine facilities.
12 Develop the capability to model small-scale mine configurations.
13. Validate (12) using experimental data from Kloppersbos, other galleries or experimental mine facilities.
14 Develop the ability to consider extended mine layouts: single entry, multiple entry, longwall mines and room and pillar.
15. Validate (14) using experimental data from experimental mine facilities or accidents.
16. Use simulation methods to develop methane and coal dust suppression methods.
17. Use simulation methods to evaluate the mine layout's effect on safety.
18. Use simulation methods to evaluate current mine safety procedures and regulations and propose modifications if necessary.
19. Use simulation methods to evaluate accidents, as required, and to assist with retrospective investigations.

These steps have been outlined to provide an overall view of a possible development path and to break the development down into realistic work packages. After the completion of a particular activity the development plan can be updated according to the most current information and, if applicable, any changing requirements.

It is also proposed that the South African Universities be involved in this development process at a more basic research level, due to their expertise and cost structure. Their developments can be incorporated in the project as they reach the necessary level of maturity. The University of Pretoria will be most suited to the development of combustion models for coal dust, and the University of the Witwatersrand should become involved in determining the dynamics of the layered dust. These universities must collaborate extensively with the relevant universities in other countries.

Close collaboration with the Kloppersbos facility will be vital in terms of developing empirical models, validation using available data, and performing experiments for further model development and validation. As much collaboration with other institutes as possible should be encouraged to ensure suitable direction and spin-off development.

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APPENDIX A: BIBLIOGRAPHY

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APPENDIX B: GLOSSARY OF TERMS

Term	Description
B-GAS	British Gas
Body-Fitted Grid (BFC)	A computational grid that has exterior surfaces which are curved to fit the obstacles in the flow field.
Boundary Conditions (BC)	Values of variables which have to be specified at the boundaries of the computational domain.
CD	Combustion Dynamics Ltd., Medicine Hat, Canada
Cells	The space between adjacent points of the grid, over which the properties are assumed to have a certain degree of uniformity in characteristics.
CFD	Computational Fluid Dynamics
CMR	Christian Michelsen Research
Computational domain	The extent of the computational simulation in space.
DDT	Deflagration to Detonation Transition
DMT	Deutsche Montan Technologie für Rohstoff, Energie, Umwelt, Germany
EM	Experimental Mine
Euler	partial differential equations for conservation of mass, momentum and energy in an inviscid fluid
FCT	Flux Corrected Transport, a CFD limiter
Grid Generation (GG)	Discretising the computational domain into a number of cells, to form a computational grid.

INERIS	Research Institute, France
MB	Mega Bytes of memory
MREL	Mining Resource Engineering Ltd., Ontario, Canada
Navier-Stokes	partial differential equations for conservation of mass, momentum and energy in a viscous fluid
PC	Personal computer
PML	Prins Maurits Laboratory
porting	adapting a computer program to a computer for which it was not originally wriiten
Rk, $k	thousands of rands, dollars
SC	Super Computer
Source	program statement text, which can be changed by a developer; in contrast to object code, which is not accessible to a developer, and is the usual form of commercial packages
Submodel	Part of a simulation model that introduces properties varying on scales smaller than the cell.
SWACER	Shock Wave Amplification by Coherent Energy Release, a mechanism for DDT
TNO	Research Institute, the Netherlands
TVD	Total Variation Diminishing, a CFD limiter
UK AEA	UK Atomic Energy Authority
UK HSE	UK Health ans Safety Executive

USBM	US Bureau of Mines
WANSW	Workcover Authority, New South Wales.
WS	Work station

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APPENDIX D: COMPONENTS OF A SIMULATION

Computer simulations of reacting flow have a number of components, into each of which is built a level of assumption about the physical processes taking place. For example, the chemistry model may consist of a system of all the reactions taking place, and assume very little about the outcome; at the other extreme, a single reaction may be written for fuel, oxidant and products, with a rate constant that hides the chemical complexity.

An apparently simple simulation is therefore generally based on far-reaching assumptions; many phenomena have been explicitly modelled. The realism of the predictions of the code depends not only on the validity of each model, but on the interactions between the models.

The alternative is to build in low-level physics, minimize the theoretical content, and allow the expected phenomena to develop as consequences of the micro-level model. This route may produce more defensible models, but generally imposes greater computing requirements.

The following are the major components required in a simulation model:

- **Fluid flow model**

Differential equations describing the flow are solved, generally on a grid of points in the volume of interest. Shock-capturing methods solve the Euler or Navier-Stokes equations; in contrast, the existence of shock or discontinuities may be assumed, and the relations across them solved together with descriptions of the intervening states (shock tracking methods). The latter method embodies more assumptions, is generally only useful in one dimension, and may require experimental correlations of flame front speed, etc.

- **Solver**

If a system of partial differential equations has been set up and discretized on a grid, there is a great variety of numerical solution methods available. This short list includes only those of immediate relevance.

- The SIMPLE finite-volume method is in wide use in combustion modelling but is inclined to smooth discontinuities; where flame-acoustic interactions, and good shock-capturing, become important, other methods have been preferred. These methods can be extended to include higher order discretisation schemes and limiters at discontinuities which make them more suitable, see van Wingerden (1994).

- Total Variation Diminishing (TVD) and Flux Corrected Transport (FCT) schemes which maintain resolution of discontinuities without introducing spurious oscillations. Combustion and turbulence closure is made more complex than when using the SIMPLE approach.
- Methods based on solutions of the Riemann problem provide excellent shock-capturing but require detailed incorporation of the combustion problem into the flow solution, and are therefore less flexible, the Godunov solver is an example.

- **Chemistry**

As described above, a one-step reaction may be formulated, or a full system solved. The latter of course requires considerable computing power, and a compromise may be reached by writing a three- or four- step mechanism.

Oran and Boris (1987) summarise a variety of methods of modelling chemistry, from simple to full systems. They have also developed as a useful compromise the induction parameter model, a two-step process dominated by the induction period of the first step, in which free radicals are produced, rather than the second, in which the radicals react.

- **Turbulence**

A number of numerical models of turbulence are available. Those which have been tried in this field include the $k-\varepsilon$ model and the PDF (probability density function) model. The former is relatively simple and widely used, but has been observed to cause numerical instability in some regimes.

- **Combustion**

The development of laminar flame fronts is relatively well-understood, but in the configurations of interest the front will be turbulent for most of the time of interest, except for local simulations. Reaction rates are then dominated by turbulent mixing rather than kinetics. Eddy break-up models have been most widely used to describe the process, but may not apply over the wide scale range necessary for large-scale simulations. Models based on statistical fluctuations of the mixture fraction have not been widely applied in the explosion field.

The techniques mentioned above are suitable for incorporation in full flow-field simulations. Flamelet models, flame-tracker methods and interface tracking methods have been used in detailed modelling of combustion fronts, but have not yet been widely applied in explosion modelling.

- **Dust**

Widely varying levels of detail are possible in the modelling of dust. Important points are summaries here.

- Separate models for coal and inert dust will probably be required.
- Dust has been modelled simplistically as a high-molecular weight gas contributing to the fuel-oxidant reaction.
- In two-phase or multi-phase models the dust has been treated as an Eulerian fluid interpenetrating the other components.
- The most detailed, flexible, and costly, models track individual particles in a Lagrangian system. This allows modelling of small-scale processes involving the particles, such as devolatilization, char combustion, particle size change, agglomeration, decrepitation, etc. Housekeeping tasks on the computing side become more expensive.
- Drag forces on dust, dust acceleration and heating, contribute significantly to combustion. Energy exchange with dust particles, including inert dust, is extremely important in modelling both combustion and quenching.
- The effect of the presence of particles on turbulence can be computed; its importance is still being assessed.
- The induction time of dust combustion may need detailed modelling in order to capture detonation correctly.
- Shock interactions with particles at the microscopic scale may affect the onset of DDT.
- Soot formation may be modelled.

Dust lifting models are widely varied:

- A very simple model may assume that the dust is uniformly initially distributed in the volume of interest.

- There have been attempts to model the lifting of dust in turbulent flow, including creep and saltation. Simple models of the formation of a dust floor layer are not common.

- **Other substances**

It may be necessary to include models for inert fluids, such as water, or extinguishers.

- **Detonation**

Given adequate shock-capturing by the flow model and solver, and a combustion model which provides accelerating flame fronts, detonation waves should be observable in the simulation system. Resolution of the interaction of acoustic modes with the front depends on good shock-capturing.

- **DDT**

The complex phenomenon of deflagration-to-detonation transition may not be realistically observed unless a specific model for its initiation is included.

- **Obstacles**

The presence of obstacles has a crucial effect on the development of turbulence and therefore flame front acceleration. Obstacles may be incorporated in a number of ways:

- cells may be blocked off in a Cartesian grid (partially porous cells);
- in an explicit method, special boundary conditions may be provided at obstacle cells (a method which has been used for cars obstructing roadways, and may prove useful for explosion-proof stoppages);
- a body-fitted grid may be wrapped around curved obstructions, but has limitations in complicated topology or with sharp corners.

- **Boundary conditions**

Boundary conditions at walls, open vents, etc. match the type of solver and the equations being solved. In complex geometries, grid blocks may be patched together and interblock boundary conditions provided.

- **Radiation**

If the presence of particles or soot formation makes the region of the explosion front optically dense, a radiation model may have to be included. The extra volume of work required, and increased complexity, make radiation a factor to be excluded from simulation unless it is essential.

- **User interface**

It is not the intention to produce functional specifications here, but the following points may be borne in mind.

- If the geometry is complex, it may be desirable to provide an interface to a CAD package or grid generator.
- Good graphical representation of the results is essential. An interface to a commercial package may be required.
- Error and help messages should be comprehensible to the level of user envisaged.
- Computer simulations of this complexity are generally not yet in the realm where untutored users can obtain useful results; the user interfaces and level of robustness may be more appropriate to the specialist than to the industrial environment.

For practical predictions, two factors are desirable:

- a high level of confidence in the results, and
- acceptable run-times and computing requirements.

The former aim points towards the use of low-level models, the latter can generally be achieved with more sweeping assumptions. However, the only way to make a decision on whether a simulation is useful or not is through test: the results of the computer program must be compared with experimental data in the regime being modelled, for conclusions drawn from computation to be built on a logical base.

Validation of computer results must therefore form an essential part of a development program. Some data suitable for validation is available in the literature, or tests may be arranged through collaborative programmes.

APPENDIX E: GAS INDUSTRY EXPLOSION SIMULATION COMPARISON

In this section, the mechanisms used in the gas explosion simulation programs, some of the applications, their relative performance in comparative tests, and their prospects for use in coal dust explosion modelling are summarised. The authors wish to acknowledge that the considerable amount of comparative work that has already been carried out enables the relative clarity of this assessment.

E.1 Christian Michelsen Research, Bergen, Norway.

Program: FLACS; $\mu - FLACS$, a scaled-down version for PCs

References: Bakke *et al.*, 1993; Bakke and van Wingerden, 1992; Hjertager 1981, 1984, 1986, 1989, 1993, van Wingerden, 1992, 1994a & b, van Wingerden *et al.*, van Wingerden *et al.*, 1993, 1994a and b; CMR product information

Fluid model: conservation of mass, momentum and energy (formulated in terms of entropy).

Numerical scheme: hybrid SIMPLE, 2nd order, fixed grids.

Submodels employed: yes.

Turbulence: $k - \varepsilon$

Flame model: flamelet, one-step combustion, tracking through 2nd order van Leer scheme in reaction progress variable equation; correction to reaction rate for thin laminar flames; turbulent burning rate employs empirical correlation; rate and viscosity from empirical correlation; team believes would predict flame speed accurately up to 1000 m/s.

Obstacles: drag coefficients based on rod bundles, burning rate enhanced at obstacles.

MERGE performance: peak overpressure closest to experiment; deteriorates at overpressures above 1.5 bar due to submodels; better for methane than propane, better for larger pipers than smaller.

Development costs: about 100 man years over 13 years, both numerical and experimental; funding from Mobil, BP, Statoil, Norsk Hydro, Exon, Elf, BMFT, Gas France.

Prospects in coal dust explosions: it is understood that the CMR team is developing a combustion model suitable for coal, based on a single phase homogeneous formulation. Results may be expected in a year or so; a water-spray model already exists.

Prospects for collaboration: To join FLACS development group about R 1.25 M over 4 years.
To obtain source code: about R 0.5 M over 4 years
$\mu - FLACS$: unknown, but source not obtainable, impeding development
Possibility of paying for a specific development in order to obtain a licence, would have to be negotiated.

Computing aspects: FORTRAN, link to CASD a CAD and input processor, post processor FLOWVIS; relatively user-friendly; runs on UNIX workstations; user group

E.2 TEL-TEK and Telemark College, Norway

Program: EXSIM, developed from FLACS

References: Hjertager *et al.*, 1992, Hjertager *et al.* 1994, Hjertager 1991, 1994.

Fluid model: conservation of mass, momentum and energy (formulated in terms of entropy).

Numerical scheme: hybrid SIMPLE, 1st order (developing 2nd order), fixed grids.

Submodels employed: yes.

Turbulence: $k - \varepsilon$

Flame model: one-step combustion, modified eddy break-up model; correction to reaction rate for thin laminar flames; turbulent burning rate not adjusted with empirical correlations

Obstacles: drag coefficients based on porous medium, burning rate not enhanced at obstacles.

MERGE performance: peak overpressure close to experiment, tendency to underpredict; deteriorates at overpressures above 1.5 bar due to submodels; better for methane than propane, better for larger pipers than smaller; flame speed validated to 150 ms^{-1}.

Development costs: after FLACS (1989), about 3 years and R 250 K; now funded by Shell and other industries.

Prospects in coal dust explosions: None at present

Prospects for collaboration: Good, possible could set up joint development where both share results. Initial access to EXSIM would have to be negotiated.

Computing aspects: FORTRAN, linked to AUTOCAD, DISPLAA, UNIRAS and AutoDESK postprocessors; runs on UNIX workstations, Convex.

E.3 TNO Prins Maurits Laboratory, Netherlands

References: van den Berg and Lannoy, 1993; Mercx, 1994; van den Berg, 1994c; van der Wel, 1994; TNO product information

Program: REAGAS; BLAST; AUTOREAGAS

Fluid model: conservation of mass, momentum and energy (formulated in terms of entropy).

Numerical scheme: hybrid SIMPLE, 1st order (developing 2nd order), fixed grids.

Submodels employed: yes.

Turbulence: $k - \varepsilon$

Flame model: modified eddy break-up model; correction for thin laminar flames; turbulent burning rate not subject to empirical correlations.

Obstacles: drag coefficients based on circular tubes, no rate enhancement at obstacles.

MERGE performance: tendency to overpredict peak overpressure, time of peak overpressure delayed due to treatment of flame initiation; deteriorates at overpressures above 1.5 bar due to submodels; better for methane than propane, better for larger pipers than smaller.

Development costs: after FLACS publications, about 8 years.

Prospects in coal dust explosions: PhD in progress at Delft University on dust lifting but not combustion; see a need for dust explosion modelling.

Prospects for collaboration: in collaboration with INERIS, France, and Poland; may be possible to collaborate economically if SA develops dust model?

Computing aspects: FORTRAN, own geometry, no CAD link; postprocessing through Autodyn, own software.

E.4 British Gas Research and Technology Division, United Kingdom

Program: $\mu - COBRA$, program from Mantis Numerics Ltd.

Fluid model: conservation of mass, momentum and total energy.

Numerical scheme: 2nd order explicit Godunov, adaptive grid.

Submodels employed: yes.

Turbulence: $k - \varepsilon$

Flame model: reaction progress variable equation; correction to reaction rate for thin laminar flames; turbulent burning rate employs empirical correlation; flame thickness imposed, grid adapted to resolve phenomena.

Obstacles: empirical drag coefficients, burning rate enhanced at obstacles.

MERGE performance: peak overpressure close to experiment, tendency to overpredict at overpressures above 1.5 bar due to submodels; better for methane than propane, better for larger pipers than smaller.

E.5 Imperial College Mechanical Engineering Department, United Kingdom

Program: GEISHA, program from Computational Dynamics Ltd.

Fluid model: conservation of mass, momentum and energy.

Numerical scheme: 2nd order TVD, fixed grids, resolves to small scales.

Submodels employed: no; resolution extended to small structures.

Turbulence: $k - \varepsilon$

Flame model: newly developed eddy break-up model.

Obstacles: resolved on grid, transients can be observed.

MERGE performance: not tested on the same basis, but used to resolve transient flow behaviour.

APPENDIX F: TECHNOLOGY/PHENOMENA BREAKDOWN

Phenomenon	Reference

F.1 Ignition phase

general development of ignition	Gaydon & Hurle (63) Jones (58) Cashdollar Michaelis, Margenburg, Müller and Kleine (87) Phillips and Landman (92)

F.1.1 Combustible properties

F.1.1.1 explosibility limits

explosibility limits, envelope, optimum explosive concentration	Gardner *et al.* (86), (85) Lee, Zhang, Knystautas(92) see also Dust Cashdollar and Hertzberg (89) Cashdollar *et al.* (92) Phillips and Landman (92) Amyotte *et al.* (88) Benedick *et al.* (86)
coal dust parameters moisture, volatiles, ash, fixed carbon, calorific value	Gardner *et al.* (86) Sichel *et al.* (85) Cashdollar and Hertzberg (89)
dust explosion constant K_{st}, cubic law	van Laar () Kjäldman (92) Phillips and Landman (92)
K_{ex}	Phillips and Landman (92)
ignition energy/temperature	Edwards,Perlee,Chaitken (77) Cashdollar

	Moen (93)
	Phillips and Landman (92)
	Benedick *et al.* (86)
	Amyotte *et al.* (88)

F.1.1.2 existing concentrations

degree of premixing

F.1.1.3heterogeneous dust mixtures

heterogeneous dust mixtures	Lee, Zhang, Knystautas
	Phillips and Landman (92)
	Amyotte *et al.* (88)

F.1.1.4 induction time

igniion delay/induction time/ZND	Sichel *et al.* (85)
	Moen (93)

F.1.2 Ignition source

F.1.2.1 mine

spark - friction - lightning - flame - spontaneous	Phillips and Landman (92)
continuous mining machine picks/coal cutter picks etc	Phillips and Landman (94)
accident data	Phillips and Landman (94)
	Amyotte *et al.* (88)
magnitude	Michelis *et al*et al (87)
shock	Sichel *et al*et al (85)

F.1.2.2 experiment

spark - pyrotechnics	Phillips and Landman (92)

jet ignition	Hjertager (81) Moen (93) Lee and Moen (80)
flame jet	Gardner *et al.* (86)
fire bed	Gardner *et al.* (86)
planar computation ignition model	Hjertager (81)

F.1.3 Oxygen

F.1.3.1 Fuel mixture

floor and roof layers	Lea (93)

F.1.3.2 Flow

flow profile	
mine layout and ventilation	
turbulence level, profile	Amyotte *et al.* (88)
duct diameter	see cell size under det

F.2 Initiation phase; unconfined explosions; vented explosions

F.2.1 Small spherical flame, development

spherical flames	[Strehlow]
parabolic flame front	Gaydon & Hurle (63)

F.2.2 Pressure disturbance development

F.2.3 Related

spherical blast waves, bombs	Barker (73)
unconfined vapour cloud explosions	Hasegawa and Sato (83)
CDE in spherical vessels	Continillo (88)

F.3 Propagation - general

F.3.1 Shock dynamics

acoustic disturbance - development of precursor shock	Jones (58) Gaydon and Hurle (63) Zhang, Greilich, Grönig (92)
blast waves, Mach reflection	Baker (73)

F.3.2 Flame dynamics

flame front velocity and acceleration - burning velocity - dependance on chemistry, activation energies, radical diffusion, heat transfer - laminar flames, (turbulent flames)	Dixon-Lewis *et al.* (87) Clark and Smoot (85) Davies (74) Lee and Sichel Gaydon and Hurle (63) Edwards and Ford (88) Jones (58) Pickles (82) Edwards, Perlee, Chaitken (77) Green Piper, Upfold (85) Bradley *et al.* (87) Lee and Moen (80) Moen, Sulmistras *et al.* (86) Hjertager (84)
reaction-diffusion front	Horvath *et al.* (73)
chaotic description	Horvath *et al.* (73)

correlations of turbulent and laminar flame velocity	Clark and Smoot (85)
turbulent effects on flame front, turbulent mixing	Clark and Smoot (85)
	Hjertager (81),(84)
	Vassart (85)
	Green, Piper, Upfold (85)
	Pickles (82)
	Edwards and Ford (88)
	Moen (93)
	Lee and Moen (80)
	Amyotte *et al.* (88)
dust flames	Clark and Smoot (85)
	Dixon-Lewis *et al.* (87)
	Davies (74)
	Amyotte *et al.* (88)
flame thickness, heat transfer through flame	Clark and Smoot (85)
	MREL notes
radiative preheating	Lee, Zhang, Knystautas (92)
tunnel temperature change, heat transfer to walls	Patrick Cook
	Clark and Smoot (85)
flamelet models	van Wingerden *et al.* (93)
	Arntzen *et al.* (94)
flame wrinkling, instabilities, flame-acoustic interactions	Lee and Moen (80)
	Green *et al.* (1993)

F.3.3 Methane explosions in particular

methane explosions	Catlin (92)
	Hjertager (81)(93)(89)(84)(93)
	Moen and Lee (82)
	Bakke *et al.* (93)
	Bakke and van Wingerden (92)
	Bakke and Hjertager (81)
	van Wingerden (92)(93)(94)
	van den Berg and Lannoy (93)
	van den Berg *et al.* ()
methane roof layers, stratification, gravity currents	Lea (93)
methane fires	Adiga *et al.* (90)

F.3.4 Chemistry and products: see modelling techniques

F.4 Deflagration-detonation transition, detonation

F.4.1 DDT

run-up distance	Lee and Sichel (86)
mechanism of DDT	Gaydon and Hurle (63)
	Jones (58)
	Zhang, Greilich, Grönig (92)
	Knystautas, Lee *et al.* (79)
	Peraldi *et al.* (86)
	Lee and Moen (80)
	Lee *et al.* (92)
	Moen *et al.* (83)
	Moen *et al.* (86)
	Moen (93)

Slow/fast stages of DDT	Zhang, Greilich, Grönig (92) Moen (93)

F.4.2 Detonation waves

detonation velocity and conditions, CJ theory	Gaydon and Hurle (63) Lee, Zhang, Knystautas (92) Jones (58) Lee and Sichel (86) Peraldi *et al.* (86) Lee and Moen (80) Wolanski *et al.* (84)
comparison of CJ with experiment	Zhang, Greilich, Grönig (92) Lee and Sichel (86)
detonation front structure	Zhang, Greilich, Grönig (92) Lee and Moen (80)
transverse waves, acoustic modes	Zhang, Greilich, Grönig (92) [Manson (47), Fay (52)] Moen (93) Green *et al*et al (93)
influence of absorbing walls, rough/smooth walls	Moen (93) Knystautas, Lee *et al.* (86)
detonation propagation in porous media	Makris *et al*et al (92)
triple points	Zhang, Greilich, Grönig (92) Baker (73) Moen (93)
spinning single-head fronts	Zhang, Greilich, Grönig (92)
two head fronts	Zhang, Greilich, Grönig (92)

retonation wave	Gaydon and Hurle(63) Jones (58)
detonations emerging from ducts	Moen (93)
Riemann problem	Jones (58)
autoexplosions, unstable detonation	Zhang, Greilich, Grönig (92) Lee and Moen (80)
SWACER mechanism - shock wave amplification by coherent energy release - chem energy realeased in manner that amps shocks	Moen (93) Knystautas, Lee *et al.* (79) Lee and Moen (80)
ZND model - Zeldovich-von Neumann-Döring 1D, induction zone	Moen (93) Shepherd *et al.* (86)
induction time calculation	Westbrook (82)
multicell det, fish scale pattern, cell size	Moen (93) Oran and Boris (87) Moen, Sulmistras *et al.* (86) Shepherd (86) Shepherd *et al.* (86) Knystautas *et al.* (83) Moen, Funk *et al.* (83) Lee and Moen (80)
turbulent pocket ignition of DDT	Moen (93)
shock collides with flame front	Lee and Moen (80)
jet ignition of DDT	Moen (93)
dust detonation	Fan and Sichel (88)

F.5 Dust and propagation

coal dust parameters	Gardner *et al.* (85)
	Sichel *et al.* (85)
	Dixon-lewis *et al.* (87)
	Cashdollar and Hertzberg (89)
entrainment, fluidisation, dust source term, saltation, surface creep, lifting	Edwards and Ford (88)
	Davies (74)
	Zhang, Greilich, Grönig (92)
	Clark and Smoot (85)
	Shirolkar and Quieroz (93)
	Mirels (84)
	Bonapace (86)
	Dawes (52)
	Dawes and Wynn (52)
	Mirels (84)
heat transfer to dust, time scales	Lee, Zhang, Knystautas (92)
	Green, Srinavas, Piper, Upfold (93)
	Zhang and Wall (93)
	Wolanski *et al.* (84)
induction time for dust	Zhang and Wall (93)
drag forces on dust	Sichel *et al.* (85)
	Vassart (85)
	Hill and Smoot (93)
ignition mechanism for dust	Sichel *et al.* (85)
	Zhang and Wall (93)
	Wolanski *et al.* (84)
	Baek *et al.* (90)
	Gururajan *et al.* (90)
	Hedley and Leesley (56)

devolatilization	Dixon-Lewis *et al.* (87) Continillo (88) Kjäldman (92) Zhang and Wall (93)
char combustion	Hill and Smoot (93) Kjäldmann (93) Magnussen and Hjertager (76) Zhang and Wall (93)
particle shrinking, swelling, agglomeration	Kjäldmann (92) Hill and Smoot (93)
supression; rock dust; quenching; dilution	Perlee and Edwards (76) Edwards and Ford (88) Johnson, Roberts, Lunn (85) Green, Srinavas, Piper, Upfold (93)
shock/dusty gas interaction	Belousov *et al* (90) Sichel *et al.* (85) Chang and Sichel (88)
CJ theory in dust mixtures	Lee and Sichel (86) Wolanski *et al.* (84)
dust explosions: general	Bartknecht (89) Li *et al.* (93) Li *et al.* (94) Van der Wel (93)
dust simulation	Chang *et al.* (87) Jones *et al.* (90)

F.6 Geometric effects

doors, fans, leakage branches	Lea (93)

2D cylindrical duct	Edwards, Perlee, Chaitken (77)
influence of duct diameter	Green, Srinavas, Piper, Upfold (91) Lee, Zhang, Knystautas (92) Zhang, Greilich, Grönig (92) Clark and Smoot (85) Moen (93) Knystautas *et al.* (83) Peraldi *et al.* (86) Moen *et al.* (82)
obstructions generating turbulence, accelerating front	Green, Srinavas, Piper, Upfold (93) Hjertager (81)..(93), (94) Baker (73) Moen (93) Moen and Lee (82) Hjertager, Fuhre *et al.* (94) Moen, Lee *et al.* (82) Moen, Sulmistras *et al.* (86)
gallery configuration	Davies (74) see also under models
tunnel intersections	Skews and Law (91)

F.7 Modelling techniques

see also model summary

F.7.1 Ignition models

ignition parameters in model	Hjertager (81) Green, Piper, Upfold (85) Lea (93)
ignition/extinction condition	Hjertager (81) (93) Proust (93)

ignition at flame front	Edwards, Perlee, Chaitken (77)
jet	Knystautas *et al.* (79)

F.7.2 Chemistry and turbulence

one-step chemistry	Green, Srinavas, Piper, Upfold (93) Vassart (85) Hjertager (76), (81) Continillo (88) Green, Piper, Upfold (85)
one-step chem, reation rates governed by turbulent mixing - eddy break-up model - Magnussen-Hjertager	Magnussen and Hjertager (76) Hjertager (81),(93) Sørheim and Hjertager () Kjäldmann (92) MREL notes
frozen chemistry	Zhang, Greilich, Grönig (92)
equlibrium thermodynamics - STANJAN	Lee, Zhang, Knystautas (92)
equilibrium chemistry	Oran and Boris (87)
comprehensive chemistry	Dixon-Lewis *et al.* (87) Clark and Smoot (85) Vassart (85) Gordon and MacBride(71) Shepherd (86) Westbrook (82) Shepherd *et al.* (86) Oran and Boris (87)
smoke, soot	Edwards (90) Magnussen and Hjertager (76) Caufield and Linden (91)

k-ε model	Green, Srinavas, Piper, Upfold (93) Vassart (85) Hjertager (81),(93),(84) Magnussen and Hjertager (76) Sørheim and Hjertager () Shirolkar and Quieroz (93)
k-ε - difficulties with grid dependence, validation	Arntzen *et al.* (94)
turbulence effect on contact surface	Green, Piper, Upfold (85) Williams (89)
other turbulence models; epxeriment	Amyotte *et al.* (88)
Taylor longitudonal diffusion coefficient	Pickles (82)
probability density function, particle adjustment in turbulence	Hill and Smoot (93)

F.7.3 Flame models: see also Flame dynamics in Propagation, solution methods below

flame velocity models in simulations	Davies (74) Lee and Sichel (86) Kurylo *et al.* (80) Pickles (82)
premixed or diffusive flame model?	Magnussen and Hjertager (76) Williams (89)
fast combustion - thin flame sheets	Williams (89)
induction time - finite flame thickness - induction parameter model	Oran and Boris (87)

premixed laminar heterogeneous flame prop code	Whiting, Smoot, Crandall (79)
flamelets	Williams (87)
flame tracking	Hirt and Nichols (81)

F.7.4 Structural loading

resolution requirements on model	Arntzen *et al.* (94)
modelling loading	Mansour and Seireg () Green *et al.* (93)

F.7.5 Code names

FLOW3D	Lea (93)
MFIRE	Lea (93)
FLACS, EXSIM,EXCAD,EXPLO	Hjertager (81)..(93) Hjertager (89)
CASD	Sørheim and Hjertager ()
REAGAS	van den Berg (94)
BLAST2D flux corrected transport	van den Berg (94)
PHOENICS 81	Kjäldmann (92)
PCGC-2	Shirolkar and Quieroz (93)
PCGC-3	Hill and Smoot (93)
CONCHAS - SPRAY	Hjertager (93)

mine network models - MFIRE	Lea (93) Edwards and Greuer (88) Edwards (90)
FLOW3D	Lea (93)

F.7.6 Solution methods, formulations

flame as moving boundary	Lee and Sichel (86)
wall boundary conditions	Green, Piper, Upfold (85) Green *et al.* (93)
Euler equations in Lagrangian form	Hasegawa and Sato (83) Oran and Boris (87)
2/3D N/S finite vol flux corrected transport algo	Green, Piper, Upfold (85) Green, Srinavas, Piper, Upfold (93) Oran and Boris (87) Boris and Book (73)
SIMPLE	Vassart (85) Hjertager (81)(85)(93) Lea (93) van den Berg and Lannoy (93) Hill and Smoot (93) Kjäldmann (92)
Riemann variables, characteristic method	Davies (74)
1D Riemann method, full real gas model and air chemistry excluding combustion	Esser (91)
Rankine-Hugoniot	Davies (74)
flame as moving boundary	Lee and Sichel Davies (74)

real gas effects	Cousteix *et al.* (94) Esser (91)
dust as high molecular weight gas	Edwards and Ford (88) Green, Piper, Upfold (85) Vassart (85)
2D mathematical model for fire spread in ventilated duct	Edwards, Perlee, Chatiken (77)
gravity current model	Lea (93)
steady state only	Hill and Smoot (93)

F.7.7 Computing techniques; hardware

parallel processing, Transputers	Green, Srinavas, Piper, Upfold (93)
Cyber 180/840	Kjäldmann (92)
Sun SparcStation 2	Lea (93)
Convex 220 + IBM RS/6000	Hill and Smoot (93)

F.8 Models

F.8.1 1D

1D tests	Clark and Smoot (85) Vassart (85) [Hjertager (82)] Green, Srinavas, Piper, Upfold (93)

F.8.2 2D

2D fire spread in duct	Edwards, Perlee, Chaitken (77)

2D oblique shock wave	Green, Srinavas, Piper, Upfold (93)
2D cylindrical duct/ignition tube	Edwards, Perlee, Chaitken (93)
2D gallery configuration	Green, Srinavas, Piper, Upfold (93)

F.8.3 3D, relatively simple

3D gallery	Green, Piper, Upfold (85) Vassart (85) Lea (93) Hjertager (81)

F.8.4 Complex configurations

ignition tube with rings	Vasssart (85) Green, Srinavas, Piper, Upfold Hjertager (93) Sørheim and Hjertager ()
tube, horizontal bar obstructions	Moen (93) Moen, Sulmistras *et al.* (86)
Norfuss 10m tube, obstructions	Green *et al.* (93)
Moura mine '86	Green *et al.* (93)
Gascoigne Wood mine	Lea (93)
vented channel	Hjertager (93) Moen, Sulmistras *et al.* (86)
vented vessel	Kjäldmann (92)
coal-fired utility boiler, steady state	Hill and Smoot (93) Ji and Cohen (92)

offshore platforms	Hjertager (91) (93) van den Berg () Bakke and van Wingerden (92) Bakke *et al.* (93) van Wingerden (92)(94)
process plants	Hjertager *et al.* (94)
fluidised beds	Ford *et al.* (93)