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HEALTH & SAFETY LABORATORY

Review of COMEX and NVBANG Explosion Models

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EXECUTIVE SUMMARY

COMEX and NVBANG are two explosion models developed by DNV. These codes are used in safety case submissions.

The information about the models is scarce and HSE Specialist Inspectors in the Offshore Safety Division 3.2 asked that HSL would critically assess the strengths and weaknesses of the models.

Information was sought from DNV, who kindly provided documents giving descriptions of the models. A set of further queries was sent to DNV, who again kindly provided answers. The developer was then sent relevant parts of the report for comments and corrections of any factual inaccuracies.

COMEX, a spreadsheet program, is a suite of five empirical models. The models in COMEX fall into two categories that are suitable either for confined geometries or for geometries with vents on all walls. COMEX must be run by an authorised person at DNV and is not available to customers on a license basis. The model constants have been calibrated against a series of experiments in enclosures, whose volumes ranged from 0.0036 m^3 to 425 m^3 – these experiments were performed between 1978 and 1983. Obstacles of different sizes, pitches and orientations can be accounted for – the obstacles are grouped into grids. The user can specify up to 20 grids that have to be identical, in terms of blockage ratio, obstacle size, etc., and the grids must be equally spaced. The constants were re-calibrated when the results from the large-scale experiments performed as part of Phase 2 of the Blast and Fire Engineering for Topside Structures (BFETS) Joint Industry Project became available. COMEX was also used to calculate the explosion-generated over-pressure for one of the tests conducted in the BFETS project.

NVBANG is a phenomenological model. The model is not normally used as a stand-alone tool; rather it is used in conjunction with COMEX or other tools that can provide an estimate of the over-pressure. NVBANG has a feedback factor that has to be tuned so that NVBANG gives the same answer as, say, COMEX. Other input parameters will have to be adjusted to account for external explosions, non-stoichiometric fuel-air mixtures, and fuels other than propane or methane, etc. NVBANG code was used to calculate the pressure time history, with COMEX providing maximum over-pressure, of one of the tests involving a propane cloud performed during Phase 2 of the BFETS Joint Industry Project.

1 INTRODUCTION

1.1 EXPLOSION MODELLING

Mathematical modelling of explosions or deflagrations is a very useful tool, either for estimating likely explosion generated over-pressures or in the investigation of an incident.

There are four levels of complexity of explosion models, from the simplest to the most complex:

- Empirical correlations
- Phenomenological models – Zone models
- Simple CFD models
- Advanced CFD models

The empirical correlations are essentially curve fits to sets of experiments – new experiments will allow the developers to re-calibrate the constants in the correlations. The correlations are easy to use and yield an answer instantly. However, the correlations are strictly only valid for the fuels studied and under the conditions the experiments were carried out. It is not known what sort of accuracy the correlations have outside their range of applicability.

A more physically realistic representation of the flow is implemented in phenomenological models. Zone models fall in the class of phenomenological models. Zone models solve a set of ordinary differential equations for each zone, with transfer of mass, momentum and heat between the different zones. There is still a fair amount of empiricism in the phenomenological models.

CFD modelling involves solving a set of highly coupled non-linear partial differential equations, i.e. equations for conservation of mass, momentum and energy. A high degree of physical realism can be incorporated the models. The distinction between simple and advanced CFD models is quite subtle, but basically involves the representation of the mesh and the combustion physics – commercial CFD codes developed specifically for explosion modelling tend to fall into the category of simple CFD models, while academic CFD codes tend to fall into the category of advanced CFD models. CFD modelling is a knowledge-based activity and places great demands on the user's understanding of a range of subjects, i.e. fluid mechanics, numerical mathematics, combustion, etc. CFD simulations are also computer intensive.

A recent review of the state of the art in gas explosion modelling was carried out at HSL, Ledin (2002) – the report is available to the public from the HSE website, from where it can be downloaded. Further details about modelling aspects can be found in the review.

1.2 LAYOUT OF THE REPORT

Chapter 2 describes the COMEX and NVBANG models in some detail; the material is drawn from the information provided by DNV's explosion modelling specialist. Chapter 3 focuses on the strengths and weaknesses of the two models, where the models are assessed along the same lines as those used in a recent review of gas explosion modelling, Ledin (2002). The conclusions and discussion can be found in Chapter 4. Chapter 5 lists the references used in the present report. Appendix A contains HSL's questions and DNV's answers – the answers are presented verbatim.

2 DESCRIPTIONS OF THE MODELS

2.1 COMEX

COMEX, COMpiled EXplosion model, can be used to calculate maximum explosion over-pressure in partially confined modules containing flammable gas. COMEX is only applicable to propane. The model is coded in an Excel spreadsheet and will run on standard desktop PCs, provided that an Excel or an Excel compatible spreadsheet has been installed. A license for COMEX cannot be purchased, but has to be run by a person authorised by DNV.

COMEX encompasses five different models – two models can be used for explosion over-pressure calculations in a confined space and three models are used for spaces with venting on all walls. The models were applicable to low two-dimensional spaces – this refers to spaces with low ratio of height to the other dimensions. There is a criterion for what constitutes a low two-dimensional space. The difference between the confined space and low two-dimensional models is that they cover different parameter ranges. Similarly the parameter ranges to which the three low-dimensional models are applicable also differ. The user should choose the model that most closely resembles the actual scenario.

Two different approaches have been implemented:

- One-step method
    - Log-log curve based on a confined space with limited amount of obstacles, a given vent area and space.
- Two-step method
    - Prediction of over-pressure in a confined, but un-congested volume taking into account the shape of the geometry and vent locations.
    - Prediction of the over-pressure amplification due to grids of obstacles

The user can specify the shape and size of the obstacles as well as the pitch, i.e. obstacle spacing within one grid, and blockage ratio. The grids are specified by the distance from the grid furthest away from the vent and the distance between grids. It is also necessary to specify the number of grids between the point of ignition and the vent area – only one vent is chosen i.e. the one expected to give maximum over-pressure. Up to 20 grids can be specified. However, all grids have to be identical, i.e. have the same number of obstacles with the same dimensions, pitch and orientation. Furthermore the grids of obstacles have to be equally spaced. This is to replicate the obstacle arrangements used in the experiments against which the model constants were calibrated.

The ignition location can be altered between central ignition or ignition at the wall furthest away from the vent opening in the box shaped room.

The constants in the five models have been calibrated against experiments in different size enclosures, ranging from 0.0036 m^3 to 425 m^3. The more than 700 experiments were carried out by DNV during the period from 1978 to 1983. Results of these experiments are not in the public domain. Briefly, the experiments were conducted in box shaped modules of various sizes. A number of different types of obstacles, i.e. pipes and boards, were introduced in the box. The largest box formed part of a rock tunnel while the others were steel boxes. Propane-air mixtures with 5.25 vol-% propane, which resulted in the largest over-pressures, and methane-air mixtures, with stoichiometric methane concentration, were used in the experiments.

The constants in COMEX were then re-calibrated to take into account results from experiments performed as part of Phase 2 of the Blast and Fire Engineering for Topside Structures Joint Industry Project, Selby and Burgan (1998).

Results from calculations of a natural gas leak using COMEX v2.0 were presented in Selby and Burgan (1998).

2.2 NVBANG

NVBANG is a phenomenological model that can be used to calculate explosion-generated over-pressures as a function of time in partially confined box shaped volumes containing a flammable gas/air mixture with vents.

NVBANG is not usually used as a stand-alone tool, but is used in conjunction with COMEX or other tools that provide an estimate of the maximum over-pressure. The calculated explosion over-pressure from, say, COMEX, is used to change a feedback factor in NVBANG so that NVBANG generates the same over-pressure. A set of parameters can then be changed to obtain the explosion generated over-pressure for other fuels, model release of relief panels, and venting of burnt gases at an early stage in the explosion. The feedback factor is coupled to the venting speed of the fuel-air mixture and needs to be increased so that NVBANG arrives at the same over-pressure as COMEX.

Vent areas, i.e. pressure relief panels, can be specified on any of the walls. The user can specify the pressure at which the relief panel opens. The program calculates the time it takes for the panel to open. It would then appear that the vents, i.e. all pressure relief panels do not have any or the same inertia. There is no restriction on maximum vent area, other than the physical dimensions of the box shaped room.

NVBANG cannot handle external explosions directly. However, COMEX can calculate the total over-pressure, i.e. including the contribution of an external explosion, so the feedback factor in NVBANG can be calibrated accordingly.

NVBANG cannot handle obstacles explicitly. Again, the feedback factor can be calibrated after an over-pressure has been calculated using COMEX.

The feedback factor is also used to take into account any increase in burning velocity due to fluid mechanical instabilities. The burning velocity is defined as the laminar burning velocity times the feedback factor.

Gas clouds with non-stoichiometric concentrations can be handled by adjusting the laminar flame speed.

A number of unit thermodynamic processes are performed at each time step, which depend on the stage of explosion.

The combustion rate or energy released is a function of the flame surface area and the local burning velocity. The expanding flame surface can assume three different shapes: a sphere, a hemi-sphere or a spherical zone. The initial flame expansion is that of a sphere. The flame expands as a spherical zone once the flame hits a wall. The spherical zone is effectively a sphere with a truncated side, top or bottom, depending on whether the expanding flame interacts first with a sidewall, the roof or the floor.

A layer of gas with thickness is burnt – the energy released in the process is uniformly distributed in the volume of burnt gas. The burnt gas undergoes an adiabatic expansion, compressing the unburnt gas until pressure equilibrium is established.

It is assumed that the vent flow is isentropic at the current pressure – the pressure equilibrium in the enclosure is then restored.

The code allows for connected volumes – to model pressure propagation and pressure piling. Dynamic opening of vents (hinged or unhinged) can be modelled. Shocks are not modelled, but their influence on the flow would be negligible provided that the flow velocity is less than 25 % of the speed of sound in the gas/air mixture, Foyn (2004). The speed of sound in the unburnt gas, assuming a homogeneous methane/air mixture at 288 K and 1 bar is of the order 344 m s^{-1}, so the effects of shocks in that part of the flow would be of importance if the velocity exceeds 86 m s^{-1} – it is unlikely that such high velocities would be generated, but it is not impossible for flows, involving highly reactive fuel-air mixtures, to attain that sort of speed in highly congested and highly confined large geometries. The speed of sound in the burnt gas mixture will probably be in excess of 850 m s^{-1}, so the critical speed is around 210 m s^{-1}, which is not untypical of a very severe explosion, but the terminal speed is very much dependent on fuel reactivity, gas cloud stoichiometry, the geometry, level of confinement and congestion, etc. This means that for high flame speed cases local shock effects could not be present, but the importance of this is dependent on the size and response time of the wall or object that is subjected to the explosion load.

The calculated pressure at time t_1 is felt immediately throughout the enclosure, i.e. like a well-stirred reactor.

The user specifies the time step size – it should normally be set to 0.001 s or 0.002 s. DNV states that it is not necessary to investigate if the solution is dependent on the chosen time step since the over-pressure has been calculated with COMEX.

The code is written in FORTRAN and can run on PCs and VAX machines.

3 ASSESSMENT OF THE MODELS

3.1 COMEX

3.1.1 Strengths

- Arrays of obstacles, via a blockage ratio, can be defined within the module;
- It is also possible to take obstacle shape and direction into account;
- Set-up of geometry is relatively fast – compared to CFD modelling;
- Short run times – compared to CFD modelling; and,

3.1.2 Weaknesses

- All obstacle arrays have to be identical in terms of number of obstacles, shape, size and pitch. This is appropriate when modelling experiments where all obstacles are the same, i.e. as in the MERGE experiments, but may not be a good representation of a typical process module on an offshore installation – with many different types of obstacles of a large range of sizes and orientations.

3.2 NVBANG

3.2.1 Strengths

- Set-up of geometry is relatively fast – compared to CFD modelling;
- Short run times – compared to CFD modelling; and
- Venting can be modelled and the relief pressure can be specified, though all vents have to have the same relief pressure.
- It is possible to have connected modules

3.2.2 Weaknesses

- It is necessary to first run another program, i.e. COMEX, to provide an over-pressure against which NVBANG's feedback factor can be tuned in order that NVBANG will give the same over-pressure;
- A number of physical processes are taken into account through adjustments of various input parameters. There is no detail information on this or how they are chosen; and
- Local pressure hot spots cannot be picked up as the module is treated as a perfectly stirred reactor where the pressure is uniform.

4 DISCUSSION AND CONCLUSIONS

4.1 DISCUSSION

The two models provide quick answers to the question of how large an over-pressure can be expected should a gas cloud ignite.

There are restrictions on the level of complexity of the geometry, i.e. number of obstacles and their physical size that can be specified. A process module on an actual offshore installation is likely to be more complex than what can be accounted for with these models. Nevertheless, these models offer the same level of sophistication as other simple explosion modelling tools and are likely to provide results broadly in line with other commercial tools. Empirical correlations tend to yield conservative answers.

It would be necessary to resort to CFD models to obtain more detailed information about the flow field, though it should be remembered that more sophisticated tools have problems too – both in terms of their range of applicability and their level of accuracy. The CFD models also place greater demands on computer resources. It takes much longer to set-up the models and run the simulations. The user of CFD must also have a thorough understanding of fluid mechanics, numerical methods, combustion, etc., more than is required with the simpler models.

4.2 CONCLUSIONS

- The two models, COMEX and NVBANG, need to be used together, though it is feasible to use a program other than COMEX to provide the over-pressure. The output from COMEX is required to adjust the feedback factor in the NVBANG model. NVBANG on its own is not intended for provision of realistic over-pressures.
- COMEX can only to be used by an authorised user at DNV and cannot be licensed. This should ensure that a consistent approach is adhered to and the user will be fully aware of the limitations of the model.
- Obstacles can be accounted for with COMEX – the obstacles are grouped in what is termed grids. It is possible to define up to 20 grids, though all grids must have identical obstacle arrangements, in terms of the number of obstacles, obstacle sizes, and obstacle orientations. Furthermore, the grids must be equally spaced. Obstacles in a process module on an offshore installation could have a more complex nature than can be represented with COMEX.

5 REFERENCES

Foyn, T. E., private communication, 2004.

Ledin, H. S., Review of the state of the art in gas explosion modelling, HSL Report No. **HSL/2002/02** (http://www.hse.gov.uk/research/hsl_pdf/2002/hsl02-02.pdf), 2002.

Selby, C. A., and Burgan, B. A., Blast and Fire Engineering for Topside Structures – Phase 2. Final Summary Report, SCI Publication No. **253**, The Steel Construction Institute, Ascot, UK, 1998.

APPENDIX A - DNV'S REPLIES TO HSL'S QUESTIONS

The questions put by HSL are presented in italic font below. DNV's replies to HSL's questions are in standard font, Foyn (2004). The questions and answers are presented verbatim.

***HSL**: Are COMEX estimated over-pressures used as reality checks - there is a statement saying that maximum over-pressure calculated with COMEX is used to obtain the "right" NVBANG pressure. Please can you elaborate on this coupling.*

DNV: COMEX is used for calculation of overpressure for propane. A feedback factor in NVBANG is adjusted to obtain the same overpressure. Thereafter, parameters can be varied to obtain the pressure for other gases as for instance methane, release of light walls or venting of burnt gas at an early stage of the explosion.

***HSL:** Can it handle external explosions, i.e. combustion of vented unburnt gases - if yes, how?*

DNV: NVBANG can not handle external explosions, but COMEX has a model for calculation of external explosions based on what we measured during our experiments.

***HSL:** It is not possible to introduce obstacles in the calculations?*

DNV: Obstacles can not be introduced in NVBANG

***HSL**: What does the code do when the spherical flame have grown to such a size that it starts to interact with the side walls, ceiling and/or floor?*

DNV: When hitting a side wall the sphere is changed to a spherical zone and when hitting the next boundary it changes to a cylindrical zone.

***HSL**: How is the time step chosen – is it specified by the user or is an automatic time step algorithm used?*

DNV: The time step is user chosen and normally 1 or 2 milliseconds

***HSL**: Is a time step size sensitivity analysis performed?*

DNV: A time step analysis is not performed since the overpressure is specified by COMEX.

***HSL**: What is the difference between the spherical shape and the spherical zone shape?*

DNV: The spherical zone is a sphere that is cut in the top and bottom if the roof or floor is hit first.

***HSL**:* *Is the increase in flame surface area due to turbulence and fluid mechanical instabilities taken into account when calculating the combustion rate?*

DNV: NVBANG increases the flame thickness to take into account increased turbulence.

***HSL**:* *How is the local burning velocity calculated – is it the laminar burning velocity?*

DNV: The local burning velocity is the laminar burning velocity times the feedback factor.

***HSL**:* *How is the thickness of the flame determined – is it derived from experiments, deduced from the burning velocity and the size of the time step, or ...*

DNV: The feedback factor is adjusted (and thus the flame thickness) to obtain the pressure given by COMEX.

***HSL**:* *What are the modelled stages of explosion – laminar and turbulent flame growth – i.e. does the model take turbulence into account, the initial laminar flame growth, the transition to turbulent flame growth and subsequent turbulent flame growth?*

DNV: The feedback factor is coupled to the venting speed of gas/air mixture and increases the flame speed to end at the COMEX pressure.

***HSL**:* *Can different vent opening pressures be specified – only relevant if more than one vent can be specified (Maximum) vent area*

DNV: Only one vent opening pressure can be specified.

***HSL**:* *Are the results from these experiments (DNV - 1978-1983) reported anywhere – are the results in the public domain, if not, what shape geometries, and obstacles, pitch, etc., were used?*

DNV: The results from the DNV experiments are not reported in the public domain. The experiments were performed in box shaped boxes of various sizes and a part of a rock tunnel. The box shape can be compared with a car garage. A variety of obstacles were used; pipes, boards, angled boards, etc.

HSL*:* *What constitutes a low two-dimensional space – criterion for aspect ratio?*

DNV: No exact criterion is given.

HSL*:* *Is the COMEX model used by DNV on a consultancy basis only or can customers purchase a software license?*

DNV: COMEX is used by DNV only. At the moment I am the only authorized user.

HSL*:* *What differentiates the two confined space models from each other and from the low two–dimensional models?*

DNV: The different models cover different parameter ranges and the model that has the most resemblance with the background experiments is used.

HSL*:* *What differentiates the three low two-dimensional models from each other?*

DNV: They cover different parameter ranges.

HSL*:* *Did the DNV experiments involve enclosures with partial fill?*

DNV: No.

HSL: *Where the DNV experiments conducted with stoichiometric fuel-air mixtures?*

DNV: The experiments were mostly conducted with 5.25 volume% propane which gave the largest pressures. Methane experiments had stoichiometric mixture.

HSL: *Is it possible to model mixtures of different concentrations - i.e. other than stoichiometric?*

DNV: NVBANG can account for different concentrations through change in laminar flame speed for the chosen concentration.

HSL: *Was propane the only fuel used in these experiments?*

DNV: Methane was used in some of the experiments.

HSL: *What is the maximum number of obstacles that can be specified in a grid?*

DNV: Number of obstacles is not an input parameter, but blockage ratio describes this type of information.

HSL: *What is the maximum number of grids that can be specified?*

DNV: 20

HSL: *Can the location of the point of ignition be altered? If not, what is the location of point of ignition?*

DNV: Ignition points are rear or central in the box shaped room.

HSL: *Can the vent area, i.e. a pressure relief panel, be placed anywhere on any of the walls?*

DNV: Vent areas are on all boundaries. The total area of the pressure relief panels is used in NVBANG.

HSL*: Is there a restriction on the maximum vent size?*

DNV: No.

HSL*: Is it possible to specify the pressure at which the vent opens?*

DNV: Yes.

HSL*: Is is possible to specify the time delay before vent opens?*

DNV: The vents open at a specified pressure and the program calculates how fast the vent opens.