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Review

Computer aided consequence analysis and some future needs

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Abstract

Computerized consequence analysis has many obvious advantages. The aim of this review is to give an overall picture of computer aided consequence analysis, computer models available and future needs in modeling. The paper consists of four important parts needed in computer consequence analysis:

- input data required for computer modelling,
- source term computer models,
- dispersion computer models, and
- hazard effect computer modelling considerations for releases of gas.

1. Introduction

The computer models for consequence analyses should be appropriate and consistent both in terms of their accuracy and in their economy of effort. It is particularly important to avoid any unnecessary use of highly complicated and time-consuming methods when the basic data to be used is of low accuracy. Therefore, in constructing the computer models, the aim has been to achieve an appropriate practical compromise between the conflicting requirements of accuracy and economy in different situations.

There are three distinct stages in estimating the potential consequences of major hazard accidents. The first is to determine the release mode and release rate of the hazardous material concerned. The second is to determine the behavior of the material after its release, and the third is to consider the effects of the material on people. Table 1 presents a summary of the main results and problems with the models employed in the different phases of consequence assessment [1].

An important feature of any of the physical models should be their ability to extrapolate from the results of relatively small-scale experiments to large-scale ones by employing hypothetical accidental releases. All models, to some de-

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TABLE 1

A summary of the main results and problems with the modelling consequence assessment [1]

Model type	Results	Deficiencies and restrictions
Discharge models	Estimated discharged amount or rate of the release Basis for evaporation and gas dispersion analyses; pressure impact of vapor cloud explosion analyses	Models are usually not applicable, if the storage pressure is lower than air pressure
Evaporation models	Estimates amount or rate of evaporated material Basis for vapor cloud dispersion analyses and pressure impact and vulnerability analyses of vapor cloud explosions	Some models are not tested against experimental data Estimation of evaporation of substance mixed with water inaccurate Stability class of weather condition is usually supposed to be neutral
Vapor cloud dispersion models	Estimates concentration as a function of distance and/ or time Basis for vulnerability analyses	Generally it is supposed that the dispersing gas cloud does not react or absorb during dispersion The topography of complex terrain is difficult to take into account Some variation in the results of heavy gas dispersion models
Pressure impact models of vapor cloud explosions	Estimates maximum pressure, impacts as a function of distance and duration Basis for vulnerability analyses	Generally it is supposed that the mixture of gas and air is homogeneous The mechanism of explosion is not exactly known Estimation of consequences of explosion is difficult in closely built areas; it is difficult to estimate impact of surrounding buildings on the dispersion of pressure waves
Heat radiation models	Estimates thermal load as a function of distance and gives information about possible influence on people and environment Basis for vulnerability analyses	Generally it is supposed that the pool is circular or rectangular Estimation of the amount of heat radiation in deflagration or BLEVE is difficult The influence of obstacles is not exactly estimated
Vulnerability models of people and environment	Estimates impacts of toxic/ flammable materials and/or pressure waves on people (or vegetation and animals)	Great variation in existing toxicity data Escape of people difficult to include Variations in the water and soil models

gree, suffer from errors arising from extrapolation, but those that the best from this point of view are those that have a sound fundamental basis and the minimum of empirical constants [2].

The aim of this review is to give an overall picture of computer aided consequence analysis, computer models available and future needs in modelling. The paper consists of four important parts needed in computer consequence analysis:

- input data required for computer modelling,
- source term computer models,
- dispersion computer models, and
- hazard effect computer modelling considerations for release of gas.

2. Input data required for computer modelling

Source emissions, meteorological conditions, and terrain can be highly variable and they must be known well in order to assure optimum performance by any model. A summary of the input data requirements usually needed in computer modelling is given in Table 2. Any given computer model will require only a few of these input data.

In most models of gas dispersion, the error in concentration prediction is directly proportional to the error in mass release rate. The source emissions model requires several pieces of input information in order to operate. A good and more detailed discussion of input information is given in Hanna and Drivas [3].

TABLE 2

Summary of input data requirements [3] (not all are required in any given model). (© 1987 AIChE, reproduced by permission of the Center for Chemical Process Safety of the American Institute of Chemical Engineers)

Required data	Explanation
Source data	Physical and chemical characteristics Geometry of source Plant operating procedures (characteristics of safety valves and plugs, control valve closing times, ventilation devices) Time variation of release rate Underlying ground surface, surface roughness Fraction of gas, liquid and aerosol
Meteorological data	On-site wind velocity Temperature, relative humidity, stability
Local area information	Local topography, including building and storage tank dimensions, dike dimensions, equipment and operating information Air exchange rates for a building Toxicological data and location of ignition sources

2.1 Some uncertainties and future needs in the input data

Modelers and field personnel should work together to develop adequate data sets for model input. For example, the heat conductivity coefficient of the ground must be known in order to be able to calculate dispersion of a cold cloud. Uncertainties in model input parameters should be quantified and the effects of these uncertainties on the model predictions assessed [3].

One of the great uncertainties in modelling is the estimation of the fraction of gas, liquid and aerosol in a release. This is an area of active research but there are difficulties in collecting experimental observations of two-phase jets and clouds.

Buildings and topography can affect the results of consequence analysis [4]. For model applications, it is clear that a topographical map of the site including building locations and dimensions is needed in the set of input data. Some analysis may be required to determine the initial dilution in the lee of the building for release at different locations for different wind directions, or for estimating the path of a dense gas flow for these conditions. There are hardly any computer models that can take into account the building effect.

3. Source term computer models

Modelling the source phenomenon for an accidental spill of hazardous material is perhaps the most critical step in the accurate estimation of downwind concentrations. Any inaccuracies in the source emission estimation will greatly influence the subsequent dispersion calculation of concentrations resulting from an accidental release [3]. Accidental releases of hazardous materials can be of many different types — gas or liquid or two phase flow, instantaneous or continuous, from storage tanks or pipelines, refrigerated or pressurized, on land or water, confined or unconfined, reactive or non-reactive. In many cases, a combination of these scenarios exist simultaneously.

Table 3 contains a list of some available source term models [5–21], which segregates model capabilities into jet release and liquid pool evaporation. This list contains only the models that have been reported in the public literature [5–21]. Only the FLJET computer model [11] treats two-phase jets, and only the Wu and Schroy [5] model treats binary-component evaporation.

3.1 Source term model comparison

Kunkel [14] has reviewed and used five different models (Ille and Springer, Army, Shell, Air Force Engineering & Services Laboratory (ESL), and Air Weather Service (AWS) model) for calculating evaporative emissions over a constant pool area for a single component. Calculations were performed by using each model to predict the evaporative emission rate for hypothetical spills of four different chemicals (N_2H_4–hydrazine; MMH–monomethylhydrazine; UDMH–unsymmetrical dimethylhydrazine; and N_2O_4–nitrogen tetroxide) [3].

TABLE 3

List of some source term models [3,11] (© 1987 AIChE, reproduced by permission of the Center for Chemical Process Safety of the American Institution of Chemical Engineers)

Model name and reference	Evaporation model	Jet model	Jet and evaporation model
Air Weather Service, AWS [6]	×		
AIRTOX [7]			×
Army [8]	×		
CHARM [9]			×
COBRA [10]			×
FIJET [11]		×	
Ille and Springer [12]	×		
Illinois EPA [13]	×		
Kunkel [14,15]	×		
Monsanto [5]	×		
Ontario MOE [16]			×
Shaw and Briscoe [17]	×		
Shell SPILLS [18]	×		
Stiver and Mackay [19]	×		
USAF ESL [20]	×		
Wilson [21]		×	

Figure 1 shows the model calculations as a function of ambient air temperature. The difference between the emission rates calculated by the models is approximately a factor of two, for ambient air temperatures above 10 °C. The AWS model predictions are independent of ambient air temperature.

Figure 2 shows the same model calculations as a function of windspeed. Again the difference between the emission rates calculated by the models varies approximately a factor of two.

3.2 Future needs in the source term modelling

Discharge models from pipes and tanks are well established for liquids and gases. Critical two-phase flow is more empirical and a large number of models have been proposed. Flash fractions for vapor may be readily calculated, but care is required in selecting the correct conditions for evaluating parameters. Estimates for liquid entrainment in flashed vapor are subject to large error. The calculation of vaporization rates of cryogenic liquid spills is also empirical. Landspill vaporization rates is thought to proceed in two phases – an initial fast rate associated with cooling of the substrate followed by a slower long term rate governed by heat transfer from the environment. Water vaporization rates per unit area are more constant, but the total is more difficult to determine as the size of the spill is hard to estimate.

In the near future, experiments will probably be concentrated on particular

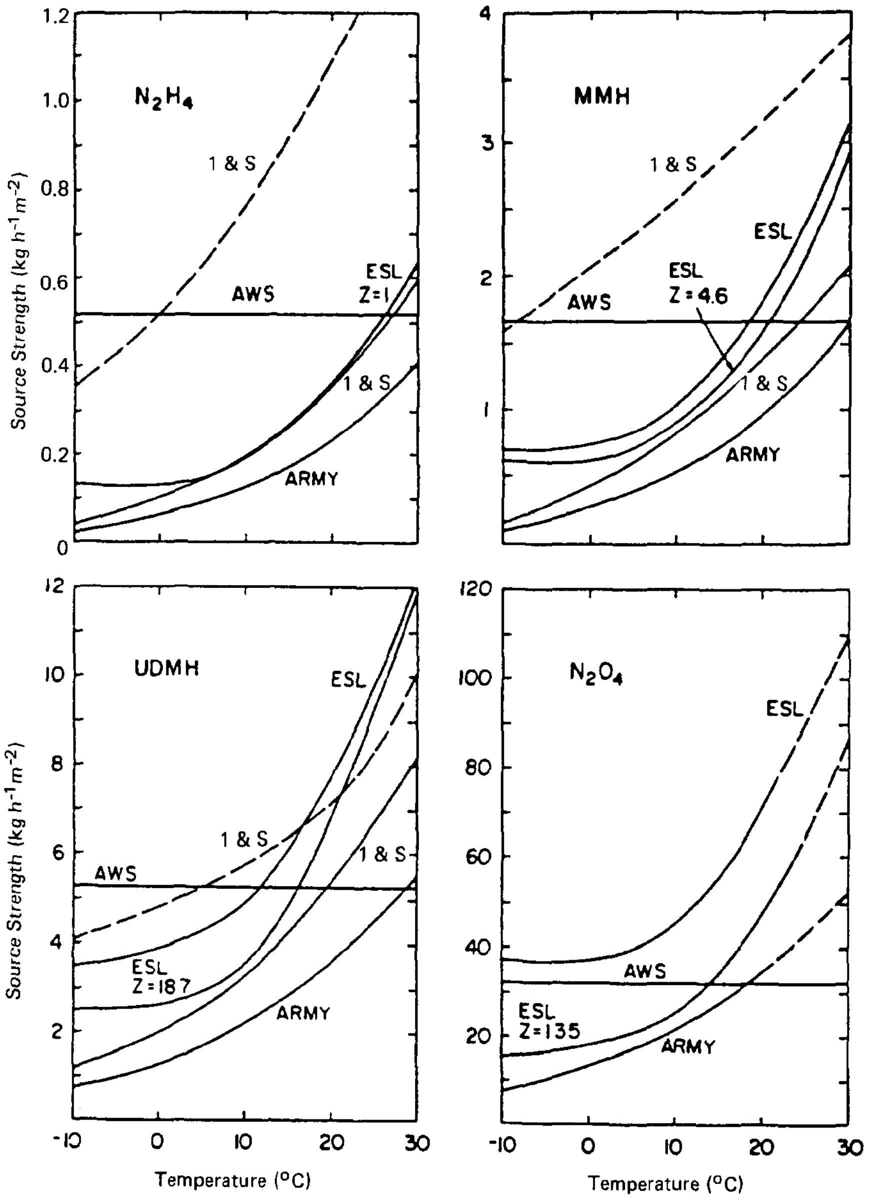


Fig. 1. Evaporative source strength (kg h^{-1} m^{-2}) as a function of ambient air temperature as determined from different models [14]. Wind speed is 2 m/s. Dashed line represents Ille and Springer model with 70° solar angle. (© 1987 AIChE, reproduced by permission of the Center for Chemical Process Safety of the American Institution of Chemical Engineers.)

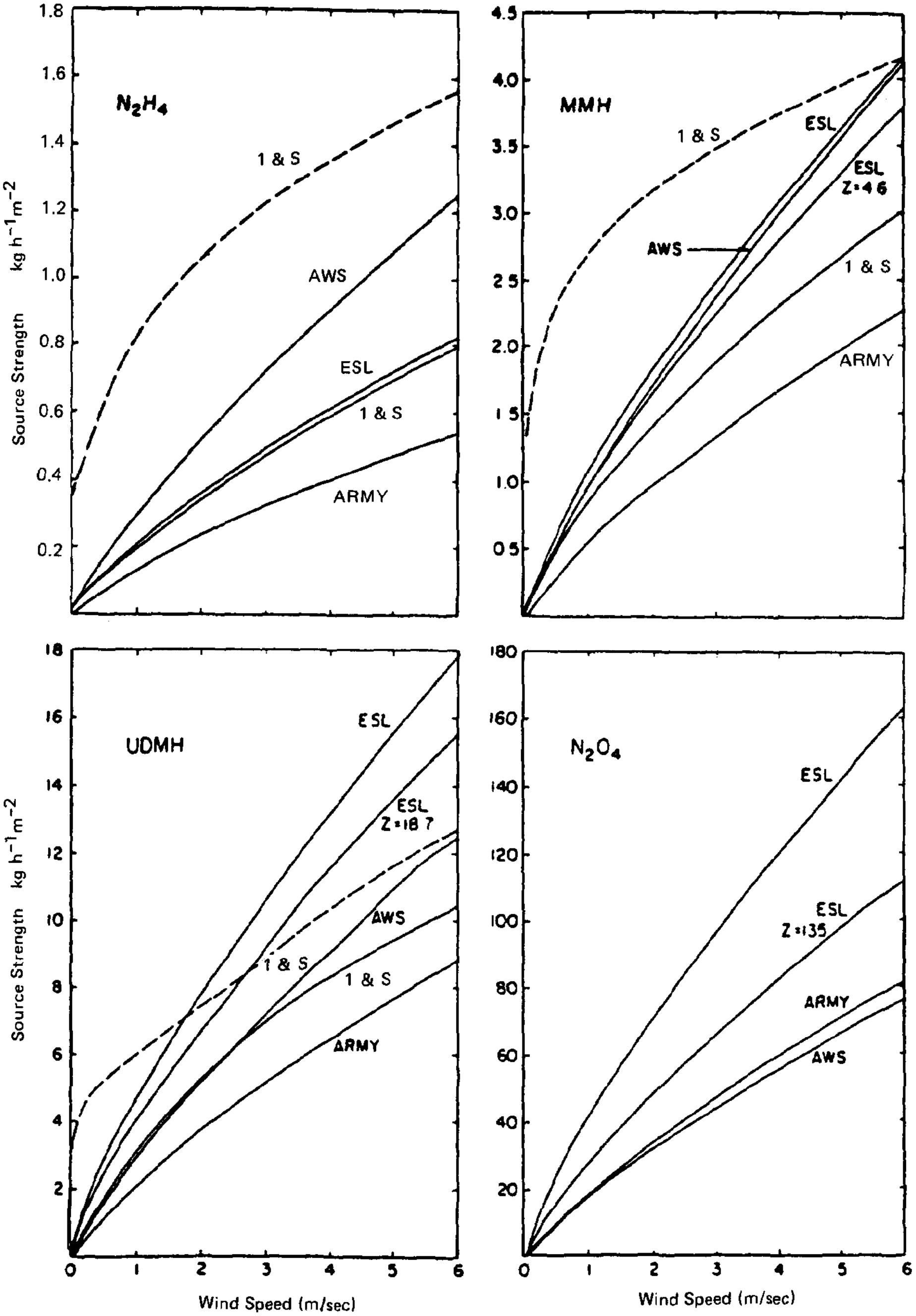


Fig. 2. Evaporative source strengths (kg h^{-1} m^{-2}) as a function of windspeed as determined from different models [14]. Dashed line represents Ille and Springer model with 70° solar angle. (© 1987 AIChE, reproduced by permission of the Center for Chemical Process Safety of the American Institution of Chemical Engineers.)

aspects of real releases, such as the nature of the source term, aerosol, humidity effects, etc. The nature of a loss-of-containment accident can influence the results of the subsequent dispersion calculation. Moreover, the releases of superheated liquefied gas can lead to considerable aerosol generation which may subsequently affect the concentration field of a dispersing cloud.

Now that well validated codes for predicting the spreading and time dependency of the vaporization of liquid spills [22] are available, the problems in this area concern:

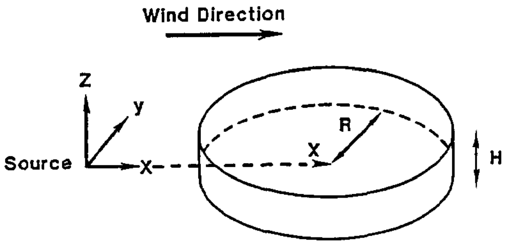
- validation and improvement of both experimental and theoretical techniques for predicting two-phase discharges from pipe networks,
- development and validation of techniques in view of the possible significance of aerosol term in dispersion calculation and the quantity of material that may be present as aerosol [23], and
- possible significance of relative humidity.

4. Dispersion computer models

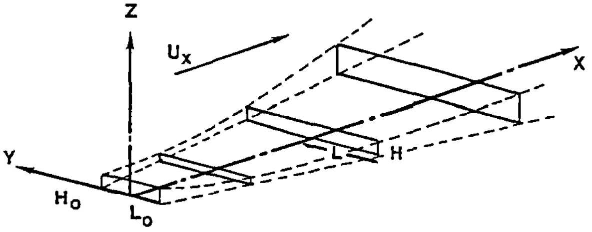
The source term models are mostly based on empirical engineering approximations to basic physical principles [3]. Only a small fraction of the source models has been adequately evaluated with field data. The situation with transport and dispersion models for hazardous materials is similar, but the number of available models is much larger. Mathematical models in concentration calculus can be classified as box, and 3-D models. In this review the box model category contains both box models and extended box models.

4.1 Box models

Table 4 contains some available box models. All the models are essentially similar in their account of gravity spreading [24], but differ to a large extent in accounting for air entrainment [25]. They are cheap to run and fairly ready to be used as an everyday tool. They are rather difficult to apply to problems involving complex terrain, calm wind conditions and time varying releases [26]. A number of box models take into account humidity and latent heat of condensation, heat transfer on the ground, differences of speed between the cloud and the wind (DENZ and Eidsvik – for instantaneous releases). Some of the models have been written for continuous releases (Eidsvik, Ooms, CRUNCH, etc. See Table 4 [7,27–58]). Box models are the most commonly used numerical models for evaluating the consequences of dispersion of denser-than-air gases in safety studies. These models assume the cloud remains a cylinder for instantaneous releases and has a rectangular concentration profile in each direction (Fig. 3). The computational time used by box models is very short due to the parameterisation of the behavior of the cloud by simple functions. The determination of the model parameters is an important issue. Difficulties arise



Cloud shape for Instantaneous Release



Cloud shape for Continuous Releases

Fig. 3. Box model cloud representation [25].

when the validation of models, considering the low number of experiments, is to be determined.

4.2 3-D models

These models use basic equations which are fair approximations and are in principle capable of accommodating non-uniform terrain and time varying releases. All existing models rely on a turbulence closure hypothesis whose validity is highly questionable. The solutions are obtained by means of numerical integration schemes which have not been separately evaluated. Table 5 contains some 3-D models [59–67].

It is therefore difficult to make judgement on the validity of the models based on such comparisons with data as have been published. The present limitations on the use of 3-D models are both practical and fundamental. Computer hardware and time requirement for a 3-D model simulation of practical dispersion problems are substantial, and the solution of such large systems of partial differential equations is complex and difficult [67].

4.3 Dispersion model comparison

Cornwell and Pfenning [68] have made comparisons of Thorney Island data with heavy gas dispersion models. From the box model group, the Cox and

TABLE 4

Some box models

Model name and reference	Dense gas	
	Instantaneous	Continuous
AIRTOX [7]	×	×
Britter [27]		×
CARE [28]	×	×
CHARM [29,30]	×	×
Chatwin [31]	×	
CIGALE 2 [32]	×	
COBRA III [33]	×	×
Cox and Carpenter [34]	×	
CRUNCH [35]		×
DEGADIS [36]	×	×
DENS20 [37]	×	×
DENZ [38]	×	
Eidsvik [39]	×	
Fay [40]	×	
Fay and Zemba [41]	×	×
Fay and Ranck [42]	×	
Germeles and Drake [43]	×	
HEAVYPUFF [44]	×	
HEGADAS [45]	×	×
HEGDAS [46]		×
Hoot et al. [47]		×
Picknett [48]	×	
Port Comp. System (MOE		×
[16,58])	×	×
RIMPUFF [50]	×	×
SAFEMODS [51,52]	×	×
SLAB [53]	×	×
SPILLS [18]	×	×
TOXGAS [54]	×	
Van Ulden [55]	×	
VAPID [44]	×	×
Webber and Brighton [56]	×	
Zeman [57]	×	×

Carpenter [34] model and the Eidsvik [39,69] model were selected. The Colenbrander and Puttock model [45] with the extensions reported by Puttock et al. [70], HEGADAS II, is an extension of the box model concept, considers concentration and velocity profiles, and uses the K-theory eddy diffusivity approach. The MARIAH II [61] model from the 3-D model group was also selected for comparison.

Figures 4 and 5 present the maximum concentrations of the various models and trial data. Figure 4 graphically presents the maximum cloud concentration

TABLE 5

Some 3-D models available

Model name	Reference
3D-MERCURE	[59]
FEM3	[60]
HEAVY GAS	[61]
MARIAH	[62,63]
SIGMET	[64]
SIGMET-N	[65]
TRANSLOC	[66]
ZEPHYR	[67]

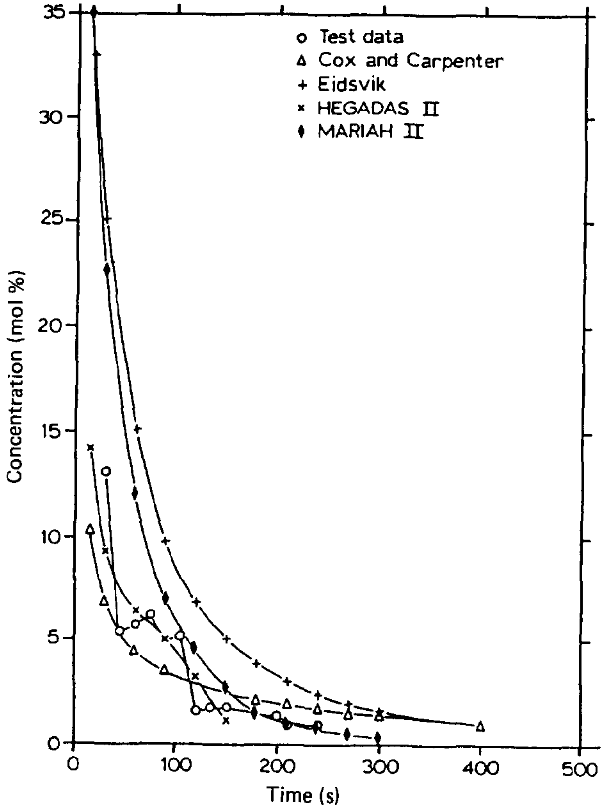


Fig. 4. Comparison of experimental results and model predictions of the maximum concentration in the cloud versus time for Trial 7 [69].

versus time for the model predictions and trial results. This picture clearly shows that the Eidsvik model significantly overpredicted the concentration of the gas cloud as a function of time. The Cox and Carpenter and HEGADAS II models both initially predicted the rate of dilution of the gas cloud fairly well. The HEGADAS II model predicted that the maximum concentration of the cloud dropped below one percent before the actual trial cloud had, whereas the Cox and Carpenter model predicted that the cloud contours had concentrations above one percent after the trial cloud had diluted below one percent. The MARIAH II initial dilution rates were similar to the Eidsvik rates. At the 120 s time interval, the MARIAH II cloud dispersed approximately as the trial cloud. In the latter part of the trial cloud life, 150 s to 240 s, the MARIAH II cloud and the trial cloud maximum concentrations matched closely.

Figure 5 shows the maximum downwind distance to the one percent concentration limit versus time for the trial and model results. This plot clearly shows that the Eidsvik model and Cox and Carpenter model overpredicted the down-

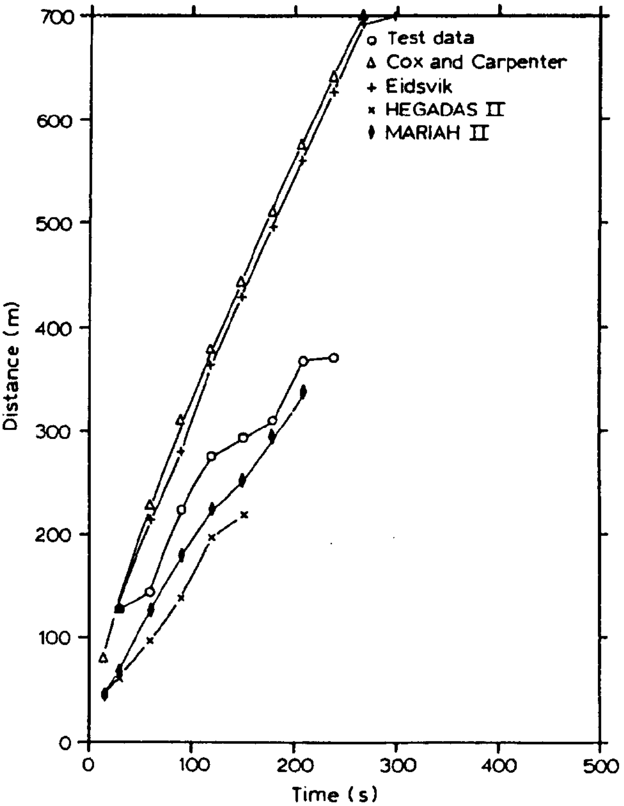


Fig. 5. Comparison of experimental results and model predictions of the maximum distance to the 1% concentration versus time for Trial 7 [69].

wind travel of the gas cloud to the one percent concentration limit. Conversely, the HEGADAS II model predicted the downwind travel of the gas cloud at this concentration level fairly well. The fact that the HEGADAS II model cloud dropped below the one percent limit before the trial cloud is also presented in Fig. 5. The MARIAH II model showed the best match of the distance to one percent concentration level as a function of time. The MARIAH II predictions closely matched the time when the cloud dropped below the one percent concentration level.

4.4 Future needs in dispersion modelling

Although current box models are adequate for assisting in decision making on problems that can be framed in a deterministic way, and useful for probabilistic assessments, there is, in the latter case, some room for a worthwhile reduction in uncertainty if more sophisticated models are developed with the following technical capabilities (cf. [23]):

- time-varying sources and transient release;
- improved top entrainment and advection prescriptions that are also valid at low wind speeds;
- improved treatment of passive dispersion and transition to passivity and definition of meteorological conditions; heat and mass transfer at the advection surface;
- aerosol effects, chemical reactions, humidity effects; obstacle effects;
- spatial and temporal variation of mean concentration and estimates of statistical variability and peak concentration.

5. Hazard effect computer modelling considerations for releases of gas

The two main hazard effects modelling areas connected with gas are its flammability and its toxicity. Exposure to toxic materials, explosion overpressure or thermal radiation are potential consequences of hazardous releases. The discussions below provide an overview of the types of hazard modelling areas in general, computer models in this field and future needs.

5.1 Toxic effect modelling

In the case of toxic materials the main concern from the emergency planning point of view is generally with the health effects of short term exposure. The inhalation of toxic gases can give rise to effects which range in severity from mild irritation of the respiratory tract to death. Lethal effects of inhalation not only depend on the concentration of the gas to which people are exposed, but also on the duration of exposure. Lethal concentrations are determined by exposing animal populations to the toxic material, and for many good biological and physiological reasons require care if extrapolated to human exposure situations.

The toxic load (TL) for a single exposure to a constant concentration may be represented by equation $TL = C^n t$, where C is concentration of the cloud, t is exposure time and n is an exponential constant.

A Probit (probability unit) function is usually used for the assessment of the percentage of the population affected. Probits appear to be a very attractive means of establishing combinations of concentration and time of exposure that will result in specific proportions of the exposed population suffering a specified level of harm. It must be pointed out that probit equations are largely based on data derived from animal population responses, and the extrapolation to human application is not straightforward.

Computer models for the estimation of toxic effects are for example SAFETI [71] and RISKAT [72]. SAFETI and RISKAT programs estimate both indoor and outdoor toxic effects.

5.2 Fire and explosion effect modelling

During the last few years vapor cloud fires and explosions have become subjects of major concern. The effects, loss of life and damage to property, have proved to be very severe. The authorities responsible for safety have an urgent need for methods and models to assess possible damage from accidental fires and explosions, so as to be able to estimate the risk of certain installations or activities such as handling, storing, and transporting combustible gases and liquids.

Different flammable substances give rise to different hazardous consequences depending on their physical and chemical properties. For example, liquefied flammable gases stored under pressure can give rise to the following hazards:

- pool or running fire,
- jet fire,
- flash fire,
- vapor cloud explosion and
- fireball or BLEVE (Boiling Liquid Expanding Vapor Explosion).

There are a great number of different methods for prediction of the consequences of explosions and fires which vary a lot both in the complexity of calculations and in the accuracy of the calculated results. Principally one may divide the prediction methods or calculation models into the following two main types: explicit analytic models and complex models.

Good analytical models can be found in references, such as TNO "Yellow book" [73] and Drysdale [74]. Mathematical computer programs for the estimation of fire effects are, for example, KAMELON [75] and for compartment fires zone models ASET-A [76], ASET-B [77].

It is convenient to group explosion effects into two types: unconfined explosions and confined explosions. The unconfined explosions occur in the open air and the confined ones within a confined space. The confined explosions may again be divided into the following two types depending on the velocity of the flame front:

- deflagrations for subsonic velocities of the flame front and peak pressure of 8 bar, and
- detonations for supersonic velocities of the flame front and peak pressure of 20 bar. Such explosions occur rather infrequently.

A computer model for an unconfined explosion is for example CLOUD [78] and for a confined explosion CONCHAS-SPRAY [79]. CLOUD contains a method for calculating the maximum overpressure and impulse for different gases. CONCHAS-SPRAY is capable of predicting effects from the most common types of explosions with a fairly high degree of accuracy.

Programs such as PC-TEMPCALC [80] and TASEF-2 [81] can be used for the calculation of response from fires and explosions. These programs are based on a finite element method. PC-TEMPCALC solves the 2-dimensional non-linear transient heat conduction equation by using rectangular or cylindrical coordinates. Composite structures and structures that enclose voids may also be analyzed. The program also includes the possibility of modelling heat transfer by convection and radiation at the boundaries of the structure. Comparisons of results from fire tests and similar calculations show reasonably good agreement. The TASEF-2 code is somewhat more user friendly than PC-TEMPCALC, but it is expected to have largely the same degree of accuracy. Generally the accuracy of the calculated results of fire response calculations depends very much on how realistic the imposed thermal heat load is specified in the input section regardless of the calculation method. Examples of explosion response codes are ADINA [82], ANSYS [83], ASKA [84] and MARC [85].

5.3 Computer models for both release toxicity and flammability modelling

Table 6 presents some computer programs for the calculation of both toxicity and flammability consequences. CASA and SAFETI programs produce risk curves in the form of individual and/or group risk. For the calculation of toxic and flammable releases risk curves the programs need information about selected failure rate cases, population distribution, ignition sources and meteorological conditions.

5.4 Future needs in toxic/flammable release modelling

The main problem in toxicity modelling arises from the possible physiological differences between animals and man, and the subsequent extrapolation of animal data obtained from homogeneous populations under controlled conditions to a highly heterogeneous human population which may be in a state of panic and exposed to fluctuating rather than steady concentrations [88,89]. When an attempt is made to combine predictions of the dispersion of vapors with toxicity data, these difficulties are multiplied because of the possibilities

TABLE 6

List of some models that take into account toxic and fire and explosion consequences

Model	Reference	Possible consequence calculation types
CASA	CASA Program System [86]	- Thermal radiation of a fireball (BLEVE) - Fire of a pool of a gas jet - Fire of a gas cloud - Explosion of a gas cloud - Explosion of a pancake-shaped gas cloud - Release of gas from container - Release of two-phase fluid - Heavy gas dispersion in the atmosphere - Dispersion of a gas jet in the atmosphere
SAFETI	The SAFETI package 1984 [71]	- Fireball or BLEVE - Instananeous pressurized release of flammable material - Continuous pressurized release of flammable material (vertical, horizontal or potentially both) - Refrigerated release of flammable material (instantaneous or continuous) - Pool fire - Instantaneous pressurized release of toxic material - Continuous pressurized release of toxic material - Refrigerated release of toxic material (instantaneous or continuous)
WHAZAN	WHAZAN [87]	- Burning liquid pool - Burning fluid jet - Exploding vapor cloud - Liquid outflow - Gas outflow - Two phase outflow - Spreading and evaporating liquid pool - Jet dispersion - Adiabatic expansion - Plume rise - Dense cloud/Gaussian dispersion - Passive plume dispersion

of escape and improvised protection, and the mitigating effects of medical treatment on human subjects.

Further experiments are needed in the fire and explosion modelling for investigating the influence of various parameters, such as: obstacles, degree of confinement, mixture reactivity and ignition location [90]. The extension of heavy gas dispersion into risk assessment for flammable gases is more complex than is generally realized, and requires greater emphasis on a more thoroughly reasoned model to interpret the effects in a more realistic manner.

6. Conclusions

Computer support is an area of intensive development. In future, better computer support is probably achieved in the qualitative tasks of a consequence analysis. Further validation studies in the field of input data, source term models, dispersion models, fire and explosion models are needed in order to achieve more reliable results.

Experiments are necessary for validation of models. More field experiments are needed to get more accurate calculation results. The recent field experiments on simplified dense gas dispersion have been very useful. Further experiments in a variety of settings that include complex terrain and sites where obstructions are present should be conducted. Experiments should also be focused on non-dense gases. The greatest need is for field experiments of tank and pipeline ruptures in which the initial acceleration is important, or in which two-phase flows are generated. Evaporation from multicomponent spills also requires field studies. The experiments should be carried out at distances where concentrations drop below the levels of toxic concern.

If major decisions are to be made as regards pollution control, evacuation plans, and risk assessments concerning hazardous gases, it is important to have the best possible information on our confidence in the models that are used and the data that are being collected. It may even be possible to build the confidence intervals (uncertainty) into the decision-making process. The total error or uncertainty in the models for source emissions, dispersion and estimation of standard deviations is composed of:

- errors generated by input data errors,
- errors caused by physical model assumptions, and
- random variability.

These components have not yet been studied in a comprehensive way. It is desirable to construct a model such that the *total* model uncertainty is minimized, because all pollutants have an impact on the environment, whether this is at short or long range.

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