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## Evaluation and Mitigation of Industrial Fire Hazards

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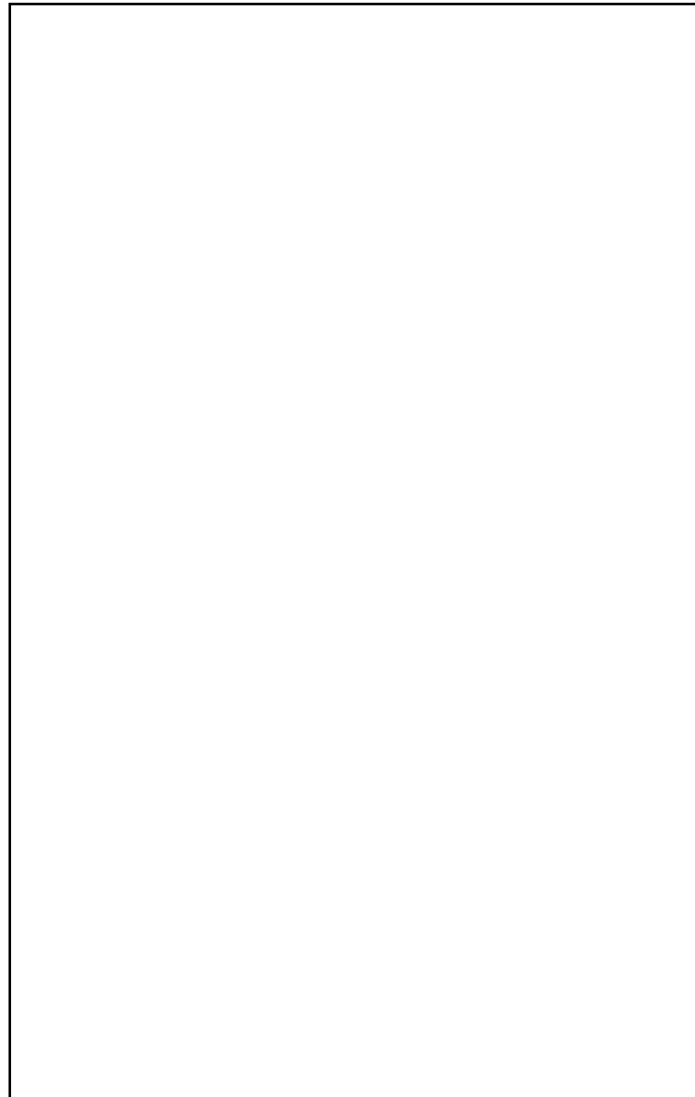
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# Evaluation and Mitigation of Industrial Fire Hazards



Petra Andersson

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# Evaluation and Mitigation of Industrial Fire Hazards

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**Keywords:** Industrial fire hazards, Smoke detection, Water mist, Halon replacement, Effect of fires, Accidental release, Human burns

**Abstract:** A tool suitable for conducting industrial fire and explosion hazard analysis is presented, together with an identification of weak links in the hazard evaluation chain. For some of the weak links additional research has been carried out.

The tool, "FREIA", evaluates the consequences for humans and components due to fires and accidental releases indoors and outdoors using established engineering methods.

Investigations have been carried out to find possible methods to simulate detector activation. The temperature, velocity, soot, CO<sub>2</sub>, CO and oxygen concentration were determined in the plume above a fire. Close agreement was found between the different compound fields. A CFD simulation of the same plume closely matched the experiments. However, there are large uncertainties involved when transforming light attenuation measurements into soot volume fraction. Simulations of tests according to the EN54 detector standard were also carried out. The agreement differed for different fuels. In addition, there is a problem with comparing light attenuation measurement performed at different wavelengths. All the results obtained indicate that it is possible to model smoke detector activation by treating the soot as an inert gas, or by assuming the soot concentration closely corresponds to one of the other compound fields. Heat detector activation is not as complicated to simulate.

The phasing out of halons often demands new solutions in order to maintain the given protection level. More recently water mist has been mentioned as a possible replacement for halons. Experiments together with theoretical considerations have shown that no presently available water mist system fulfils the requirements of a total flooding system. A narrow window exists, however, in which a water mist can function as a total flooding system. Several halon-like agents have been developed. These, however, produce more thermal decomposition products than halons, the amount produced was found to be proportional to the amount of fuel burnt in the presence of the agent. In addition, experiments have shown that they can actually increase the fire instead of extinguishing it, if not properly designed.

Estimating human burns is difficult; a test dummy for such measurements is presented.

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Front page photo: Full-scale water mist experiments carried out in Karlskrona 1996.

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Dimma



## Errata in "Evaluation and Mitigation of Industrial Fire Hazards"

Paper VI, page 11, line 7, reads ... "droplets monitored will be less than 20  $\mu\text{m}$ "  
should read ... "droplets monitored will be less than 50  $\mu\text{m}$ "

Paper VII, equation 1 should read

$$\Delta T_{(x,t)} = \frac{Qx}{k} - \frac{8Q \cdot l}{k \cdot \pi^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2} e^{-\frac{\alpha(2n+1)^2 \pi^2 t}{4l^2}} \sin \frac{(2n+1)\pi x}{2l}$$

same paper, page 5, line 11, reads "temperature of about 28-35°C"  
should read "temperature of about 28-34°C"

same paper page 7, line 4 from bottom of page, reads ... "i.e. 5-9°C above a"  
should read ...i.e. "3-9°C above a"

Paper I has now been published in Journal of Loss Prevention in the Process Industries, Vol. 10, No. 4, pp. 265-269, 1997

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## List of Papers

Included in this thesis are seven papers published or submitted for publication in international symposiums or fire safety journals. These papers are listed below together with other publications related to this work but not included in the thesis.

### Papers included in this thesis

#### Paper I

"FREIA - An expert system for fires and explosions in the process industries"

Petra Andersson, Björn Karlsson, Sven Erik Magnusson and Göran Holmstedt

Accepted for publication in *Journal of Loss Prevention in the process industries*, 1997.

#### Paper II

"CFD-Modelling Applied to Fire Detection - Validation Studies and Influence of Background Heating"

Petra Andersson and Göran Holmstedt

10. Internationale konferenz über Automatische Brandentdeckung, *AUBE '95* held April 4-6 1995 in Duisburg, Germany, pp 429-438.

#### Paper III

"Experimental Studies and CFD Simulations of a Fire Plume for the Prediction of Smoke Detector Activation"

Petra Andersson, Sören Isaksson, Zenghua Yan and Göran Holmstedt

Submitted to *Fire Safety Journal*, 1997.

#### Paper IV

"Investigation of Scale Effects on Halon and Halon Alternatives Regarding Flame Extinguishing, Inerting Concentration and Thermal Decomposition Products"

Göran Holmstedt, Petra Andersson and Jan Andersson

*Fourth IAFSS, Ottawa 1994*, pp 853-864.

#### Paper V

"Limitations of Water Mist as a Total Flooding Agent"

Petra Andersson and Göran Holmstedt

Submitted to *Journal of Fire Protection Engineering*, 1997.

Paper VI

"An Instrument for Determining the Total Water Content in Air whilst Extinguishing Fires"

Petra Andersson and Göran Holmstedt

Submitted to *Fire and Materials*, 1997.

Paper VII

"Heat Sensing Manikin Test Probe"

Petra Andersson and Göran Holmstedt

Submitted to *Fire and Materials*, 1997.

Other related publications not included in the thesis

"An Expert System for Fires and Explosions in the Process Industries"

Petra Andersson, Björn Karlsson and Sören Isaksson

*Fourth Nordic Workshop on Use and Development of Numerical Fire Models*, Kollokole Denmark September 3-4, 1992.

"Natural gas - Safety level - Risk analysis" (in Swedish)

Berit Andersson, Petra Andersson, Göran Holmstedt and Stefan Särdaqvist  
*LUTVDG/TVBB-3073*, Lund 1994.

"CFD simulation of activation of smoke detectors"

Petra Andersson and Göran Holmstedt

*First European Symposium on Fire Safety Science*, ETH Zürich, August 21-23, 1995.

"Small scale experiments and theoretical aspects of flame extinguishment with water mist"

Petra Andersson, Magnus Arvidson and Göran Holmstedt

*LUTVDG/TVBB-3080*, Lund 1996.

"Full scale extinguishing tests using different water mist systems in a 50 m<sup>3</sup> container in Karlskrona 26/8-29/8 1996" (in Swedish)

Petra Andersson and Göran Holmstedt

*LUTVDG/TVBB-3089*, Lund 1996.

"A users guide to GASOL" (in Swedish)  
Berit Andersson and Petra Andersson  
*LUTVDG/TVBB-3084*, Lund 1996.

## Nomenclature

A	frequency factor, mole <sup>1-a-b</sup> /s
a	area, m <sup>2</sup>
b	constant for potentiation of CO from CO <sub>2</sub>
C	concentration, ppm or g/m <sup>3</sup>
c	specific heat of gas at constant pressure, kJ/kg/K
d	constant for potentiation of CO from CO <sub>2</sub>
E	heat flux dose, J/m <sup>2</sup>
E <sub>a</sub>	activation energy, J/mole
F	view factor, dimensionless
f	fraction transferred to fuel surface
FED	Fractional effective Exposure Dose
g	acceleration due to gravity, 9.81 m/s <sup>2</sup>
h	heat transfer coefficient, W/m <sup>2</sup> /K
H <sub>c</sub>	heat of combustion, J/kg
k	reaction rate constant, mole <sup>1-a-b</sup> /s
k	thermal conductivity, J/m/K
L <sub>c</sub>	heat loss factor, dimensionless
L <sub>v</sub>	heat of gasification, J/kg
m	mass, kg
$\dot{m}$	mass flow, kg/s
P	pressure build-up in room, Pa
$\dot{q}$	heat release rate, kW
q"	heat flux, W/m <sup>2</sup>
R	gas constant, = 8.3143 J/mole/K
T	temperature

t	time, s
u	velocity, m/s
V	volume, m <sup>3</sup>
z	height, m
⋮	emmissivity
	density, kg/m <sup>3</sup>
	Stefan Boltzmann constant, = $5.67 \times 10^{-8}$ W/m <sup>2</sup> /K

subscripts

∞	ambient
0	initial
c	convective
comp	component
cr	critical
d	damage
E	external
eff	effective
f	flame
g	gas-layer
gm	gas mass
L	loss
o	opening
r	radiative, received
s	surface
tot	total
w	wall

## **Overview**

In the first chapter of this thesis an introduction to and background of the problem is presented. It discusses why industrial fire safety has become of increasing importance and also how industrial fire risk analysis should be conducted, in order to meet the demands of both society and industry.

When conducting a fire or accidental release risk analysis several evaluation steps are required. One major part is conducting hazard analyses, these, together with the statistical treatment of the hazard evaluation, produces the risk analysis. This thesis concentrates on the hazard evaluation in industry.

A hazard evaluation chain starts with an initial event. When the initial event is chosen the progress of this event must be decided. If the initial event was a fire, then the fire can continue to grow, or be extinguished if the fuel or oxygen are exhausted, or it can be extinguished, or suppressed by an extinguishing system. The consequences of an accidental release can be decreased by an automatic closing system, or by removing all ignition sources, etc. Together with automatic extinguishing, or closing systems, a detection system is required to initiate the protection devices. Once the progress of the fire, or the accidental release, has been predicted the consequences for people and equipment in the vicinity can be evaluated.

Chapter 2 presents a computer package suitable for conducting hazard analyses of industrial plants, which concentrates on the fire, explosion and accidental release of toxic and/or flammable substances. This package called FREIA is also described in Paper I. FREIA has been developed for use in risk analysis of both operating industrial plants and those being planned. During the development of and, to some extent, the use of FREIA, several weak links in the risk evaluation chain have been identified. Further research has been conducted into some of these and the results are presented in chapters 3-5. Some problems which have not been investigated are only briefly mentioned.

The problem of detection is discussed in Chapter 3. To initiate an automatic protection system some detection system is required. Fires are most commonly detected using heat and smoke sensitive devices. It is possible to predict the activation of a heat detector using Computational

Fluid Dynamic simulations or, for simple geometries, by the use of ceiling-jet theory. However, predicting smoke detector activation is much more complicated. Paper II and III presents some ideas for evaluating smoke detector activation.

The use of extinguishing systems are discussed in Chapter 4. A particularly important reason that such systems have become an area of increasing interest is due to the phasing out of halons. No replacement agent has yet been found which could replace halons in all situations. When replacing halons, the required fire safety level must be considered, together with other factors, such as are people present in the room and the available storage volume for any extinguishing agent. Halons are usually replaced by fire prevention measures such as vents, detection systems, etc., rather than by a new agent. When replacing with another agent there are two possible approaches, replace it with a halon-like agent or by some other agent. Some of the problems with halon-like agents and general testing of agents are discussed in Paper IV. Water mist has recently been considered as a possible halon replacement. However, there are presently no design codes available for such systems. To develop appropriate design codes, it is essential to be able to measure the water content in the air produced by the water mist. The details of a suitable instrument are described in Paper VI, while the problems of water mist as a total flooding agent are discussed in Paper V.

The last link in the hazard evaluation chain is probably one of the weakest. Namely the evaluation analysis relating to the overall consequences of a fire or an accidental release. This would include the effect of the fire and the accidental release on humans, the components and the environment, as discussed in Chapter 5. In FREIA a rather simple approach for evaluating the effect of heat on components is used, because no other appropriate model is presently available. To develop a better model further research and development are required. A human skin simulator constructed to evaluate burns on humans in fire and extinguishing scenarios is discussed in Paper VII. The toxic and pressure effects on humans, the environment and components are briefly mentioned in Chapter 5.

Chapter 6 concludes this thesis and presents some suggestions for further work.

# 1 Introduction

In Sweden 100 to 150 people die annually in fires. The direct cost of the damage caused by fires amounts to 3-4 milliards SEK per year. If the costs due to the interruption, fire prevention and fighting are included the total costs increases to approximately 12 milliards (1992). The total number of fires is 30-35000 per year. If a ten year period is considered, the large fires which represent only 1% of the total number are especially expensive as they represent 50% of the total costs. With fires in trade, industrial and construction sector representing 75% of these costs.

Fire safety issues are becoming increasingly important in modern society, as it is characterised by complex production and communication systems, by the development of new materials, by the dense storage of highly valuable goods, and by the handling and storage of hazardous chemicals. To this, we can add an enhanced awareness of risks and also the unwillingness of society, as well as industry and insurance companies to accept the high risks entailed. Increasingly more expensive precautions are therefore being included in all sectors of the society to mitigate these fire risks. The risk of dying in a fire as compared to other risks in Sweden, is detailed in Table 1.1. As seen the risk is small compared to the risk of smoking and other risks taken voluntarily.

Table 1.1. Comparison of the risk of dying.

Activity	Risk per person and year
Accidents in general	$5 \times 10^{-4}$
Traffic accident	$1 \times 10^{-4}$
Fire	$1 \times 10^{-5}$
Lightning	$1 \times 10^{-7}$
Motorcycling	$1 \times 10^{-3}$
Smoking (1 pkt/day)	$5 \times 10^{-3}$

The Swedish National Rescue Services Board (SRV) has recently studied general trends regarding risks in the society. They concluded that society becomes increasingly more vulnerable to disturbances in services associated with electrical power, telecommunications, transportation and industrial production. The risk potential increases in industry, such that even small accidents can cause significant problems in terms of the interruption of

delivery and lost market share. US statistics show that 40 per cent of the small business that have had a major fire never reopen. Larger and more complex buildings, and new materials can lead to more severe fires, where the increased hazards are difficult to foresee. New risks are introduced by new chemicals, and also by transportation and handling of hazardous materials. The increasing risk of sabotage and violence must also be considered. Environmental risks due to release of toxic products and smoke will also probably increase. Finally, it must be remembered that the nuclear power plants will remain in operation several years into the next century, representing a significant hazard, if not appropriately managed.

The development of complex systems makes society even more vulnerable and safety issues therefore become of strategic interest. Complex systems are sensitive to disturbances and even small incidents can seriously threaten life, property and environment. Large systems are difficult to survey and the function of the various components difficult to appraise in accident situations. In addition, they are difficult to control in unforeseen situations and also vulnerable to sabotage. On the other hand, complex systems have much to offer in economic terms if the associated problems can be overcome.

Today's industries are complex systems. They usually contain several components, or parts, which cannot be allowed to lose functionality, unless a substantial financial, or human loss is acceptable. For instance, in nuclear power plants one cannot afford to lose control over the reactor. In less dangerous sites it is also very important to be able to control the production process, in for instance power or chemical plants. The result of a loss in control may not always be the loss of life, it could be the destruction of material, or the production of a substandard product. All of which could be very costly for a company due to not only loss of material and products, but the company could also be sued, or, at least lose goodwill and market share, if a defective product is marketed. Insurance companies cover the losses due to the fire in for instance new plant, materials and machines, but not the loss of market share.

Many industries are very dependent on the function of a single machine. If this is destroyed, or loses functionality then the production can be stopped. Some machines are so complex that it takes years to replace them, during such time, the company will of course lose their market share and possibly never reopen. To lose functionality of some of these parts may

not require a severe fire, a small fire starting at a vulnerable location is sufficient.

Production time is also very important. This means industry is even more vulnerable to interruptions in production, especially as many only maintain minimal storage schedules, i.e. adopts "just in time" production. This could mean for instance that if car steering wheels are not produced for two weeks, then no cars can be delivered either for two weeks. Two weeks loss of production could be enough to force the company into bankruptcy. It is also common that production of a certain component in a larger system is concentrated at a certain factory, this could make the production process even more vulnerable.

New synthetic materials are constantly being developed. They may have excellent properties, but often their fire performances are decisive as to whether or not they can be used in practice. The traditional method of evaluating them has been to carry out fire tests to determine their particular fire properties. The results obtained have then been used to rank materials based on a few parameters. Unfortunately the real fire performance is often poorly predicted by many of the traditional test methods, which are not usually based on sound scientific and engineering principles. Better predictive tools could be provided by combining fire modelling approaches with modern testing technology. Thus theoretical analysis can be used to evaluate the danger associated with the burning of particular materials, products, or combinations in various scenarios. In industry, new substances and technical solutions are constantly being used, it is therefore impossible for fire safety codes to keep up. It is also well known that many fire safety systems are simply out of order, for instance if the plant has been in operation for a while fire doors are often left open, or materials are stored above the sprinkler heads.

Fires can be devastating for the environment. Large quantities of toxic gases are produced by incomplete combustion and often the debris of unburnt fuel and extinguishing media contaminates the local environment as well as more generally. The Sandoz disaster in 1986 is an example of such an accident, where the entire river Rhine downstream from the fire was severely polluted.

The building sector has by tradition been highly regulated by prescriptive regulations. In connection with the European harmonisation such building regulations are being reformulated into performance based requirements.

This allows architects and building designers to solve fire safety of buildings, in new and cost effective ways, provided of course the appropriate knowledge of fire behaviour is available. With the introduction of advanced fire engineering significant cost savings are within reach even in a short time span.

All this calls for new ways of evaluating the fire safety of industrial plants. One would like to be able to evaluate the safety of humans both inside and outside of factories, as well as, the safety of certain components inside the plant and the environment outside the facilities. Human and environmental safety is a demand from society and the safety of certain components is essential, in order to keep the production going and retain market share.

In this thesis a possible tool for such analyses is presented, together with the weaknesses of the approach and the evaluation process. In certain areas, such as fire detection and extinguishment, research has been carried out in order to improve the evaluation process.

## **2 A Tool for Conducting Industrial Fire and Explosion Hazard Analysis**

A possible tool for evaluating the fire safety of an industrial plant is FREIA. FREIA stands for (industrial) FiRe and ExplosIon hazard Analysis. FREIA evaluates the consequences of fires and the accidental release of hazardous substances inside and outside of buildings based on well established models. An overview of FREIA is presented in Paper I.

The main object of FREIA is to function as a tool for fire protection engineers in designing and analysing risk at power plants. FREIA treats fires and the accidental release of toxic and/or flammable gases and liquids, such as natural gas, propane, chlorine, ammonia, gasoline, etc. It can therefore be used in various types of industry. Stored gases may be condensed either by pressure, or cryogenically. The system runs on a PC using DOS.

FREIA has four main advantages compared to other computer programs which evaluate the consequences of fires and accidental releases:

- It considers both conventional fires, such as fires in cable trays, and also accidental releases. It also takes into consideration the interaction between fires and the accidental release. For instance, the initial fire can result in an accidental release.
- Release both inside and outside a building are considered.
- The program is an expert system. This means that even if it is not possible to calculate the consequences in detail, general advice is given to the user. If, for instance a gas release strikes a wall, or the floor, then it is not possible to deterministically calculate the concentration field close to the release. The user will, however, obtain the expert system's estimate of the concentration at the location.
- It considers damage to components.

### **2.1 System design**

The FREIA evaluation part is in principle divided into two, namely the fire and the accidental release parts, with each built using well known validated models. The two are, however, interdependent. On starting an

evaluation, the user has first to decide if the fire, or the accidental release is the initial event. Some help on choosing an initial scenario is provided by the statistical database which contains statistics on ignition and accidental releases.

FREIA calculates the consequences for both humans and components in the vicinity of the fire and/or the release. The system includes the impact of the active control systems, such as sprinkler suppression, explosion relief vents, smoke ventilation, gas and smoke detectors and carbon dioxide extinguishant. Humans and components can be affected by heat, pressure and toxic gases. For scenarios inside buildings, the result of an evaluation is presented as the estimated ratio between the heat experienced by the component and its failure criteria. The geometric positions of the components in the room are considered, but not shadow effects. For scenarios affecting areas outside buildings, the repercussions on humans are considered to be of paramount importance. It is also possible, if the user prefers, to observe results for a specified component. However, a significant lack of data on when components become damaged has been revealed and therefore only rather crude models are used to estimate the time to component damage.

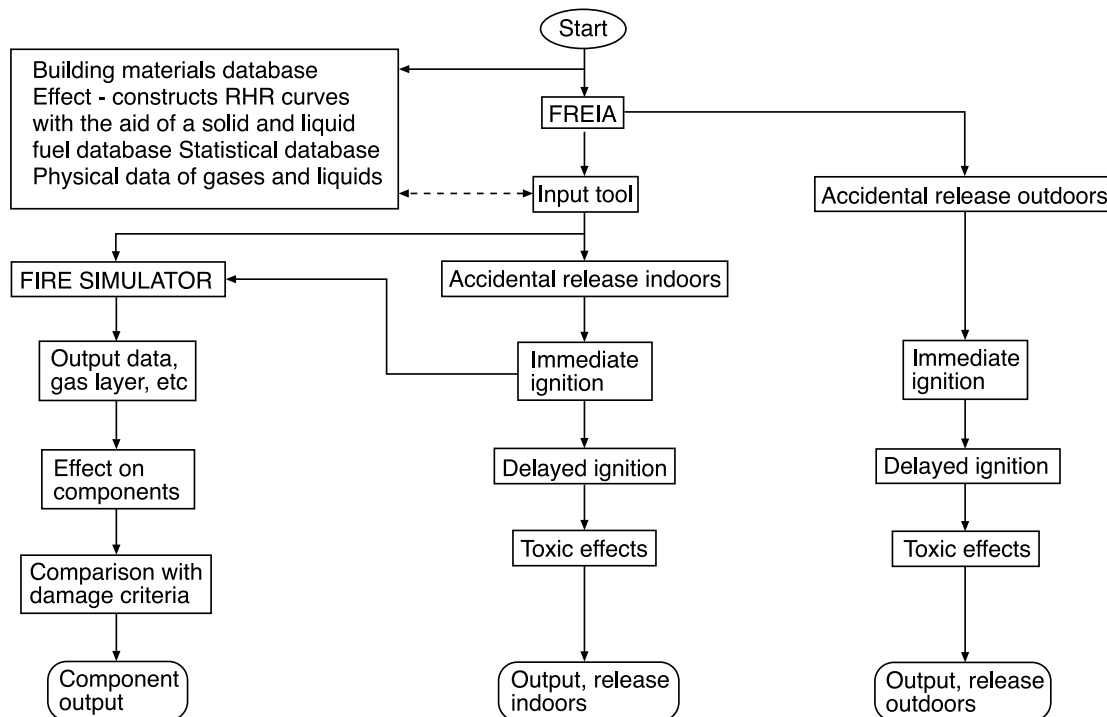


Figure 2.1 The flow chart of FREIA

The general design of FREIA is presented in figure 2.1. The system contains a pre-processor for creating input data for the system, as indicated in the figure. This pre-processor includes databases of building materials, fire response, physical data of gases and liquids, the fire characteristics of liquid and solid materials, damage criteria of components and also one database, with statistical data on accidental release and ignition. All these databases can be edited by the user. The pre-processor also includes a tool for preparing input data files for a specified room.

## 2.2 Fire in a compartment

The calculation procedure within the system for fires in compartments is divided into two categories: models which calculate environmental parameters, such as hot layer temperatures and those which estimate the effect of this new environment on the components.

Scientists at NIST have developed a computerised package of relatively simple engineering equations and a model called FPETool [Nelson, 1990]. Part of this package is a simple two-zone model called FIRE SIMULATOR which is used to calculate the environmental parameters in the fire part of FREIA.

FIRE SIMULATOR solves two simultaneous differential equations, based on the concept of conservation of energy and mass, to compute the temperature and volume of the smoke layer produced by a prescribed rate of heat release. One equation calculates the increase in temperature considering the energy input, the energy losses and also the air entrained by the rising plume. The other calculates the rate of descent of the smoke layer, as a function of the temperature increase and the rate of mass flow in the rising plume, at the point where it meets the descending smoke layer.

Several other calculation procedures are linked to the differential equations to take account of vent flow, heat losses to walls, the effect of oxygen concentration on rate of energy release, heat and smoke detector response, mechanical ventilation and also many other physical processes. Additionally, certain modules from FPETool are used to present the results graphically, help the user to define an energy release rate, help the user to build and use databases, etc. The concentration of unburned

hydrocarbons leaving the enclosure is also calculated, thus allowing the risk of the fire spreading to an adjacent compartment to be estimated.

The two differential equations based on the conservation of mass and energy which are solved in FIRE SIMULATOR, do not take account of any potential dynamic pressure build up in a room. When a fire starts in a room there will be some increase in dynamic pressure due to the thermal expansion of gases. In some cases, especially rooms with small openings, or leakage areas, an increase in pressure may cause windows to break, or other building elements to fail. It is therefore important to try to estimate the magnitude of dynamic pressure increase.

The amount of energy released in a fire will depend mainly on the amount of oxygen available and on the quantity and type of fuel. The efficiency of the combustion will to a considerable degree also depend on these factors. This will, in any case, not be complete and unburnt gases will be present. In certain cases, especially in compartments with small openings, the concentration of unburnt gases will exceed their lower flammability limit in air, thus creating a potential explosion hazard if air/oxygen are suddenly introduced into the room. It is therefore important to estimate the quantity of unburnt gases generated in a room fire.

FIRE SIMULATOR does not in fact expressly calculate these quantities. An auxiliary program AFTER was therefore written to perform such calculations. AFTER reads the input file and also the results from FIRE SIMULATOR and performs the calculations according to the procedures detailed below and then displays the results graphically.

### 2.2.1 The pressure changes

A simple mass and energy balance can be set up for a room with a certain leakage area at the floor level. Assuming that the only energy lost is by heat transfer to the walls and ceilings (the hot gases are not lost through any openings) the equations can be solved analytically to produce the following expression for the pressure build-up P (assuming the quasi-steady state) [Zukoski, 1978]:

$$\Delta P = \left( \frac{\dot{q}(1-L_c)}{cT_o a_o} \right)^2 \cdot \frac{1}{2\rho_o} A \quad (2.1)$$

where  $\dot{q}$  is the rate of heat release,  $L_c$  is the heat loss factor,  $c$  is the specific heat at constant pressure of the gas,  $a_o$  is the leakage area or the opening area,  $T$  is the temperature and  $\rho_o$  is the density. The subscript "o" refers to the gases being expelled out through the opening. The leakage area is assumed to be situated at floor level and the gases are therefore at ambient temperature.

### 2.2.2 Formation of unburnt gases

Excess fuel (that which is generated in excess of the oxidation capacity of the available air) is monitored as a potential energy source. When the room is closed the excess remains inside. When there is an opening, the excess is considered to flow out and is then added to the energy in a special fire data file. This fire data file is then available for use in estimating the impact of the fire on an adjacent room, or space, or for estimating the extent of flame from any opening.

AFTER uses the information in the fire data file, as well as, the calculated mass flow of gases through the opening, to calculate the mass of unburnt fuel per cubic metre of gases flowing out. The fire data file reports the mass of unburnt fuel (as g/s) and the modified FIRE SIMULATOR output file reports on the quantity of gases flowing through the opening in cubic meters per second. The quantity of unburnt gases (as  $\text{g/m}^3$ ) is thus calculated by dividing the former by the latter. If the quantity of unburnt gases exceeds  $45 \text{ g/m}^3$ , then it is assumed that the lower flammability limit has been reached and there may be a risk of an explosion or more often a flashover, if oxygen is suddenly introduced into the gaslayer.

The above methodology can be used to estimate time to flashover in a compartment and also the risk of a second one becoming involved. In addition, the time to detector, or sprinkler activation, or the time to damage of critical components, such as pumps and electrical cables, and the influence of mechanical ventilation and smoke relief vents, etc. can be estimated. Such information can then be used by engineers as an aid to decisions involving which fire protection measures should be implemented in power plants and other industrial installations.

## 2.3 Accidental release

The accidental release part of FREIA includes both continuous and instantaneous releases of toxic and/or flammable gases and liquids, both indoors and outdoors. Substances which are in the gas phase at room temperature and normal pressure can be condensed either by pressure or cooling. Substances in liquid phase at room temperature and normal pressure can also be pressurised or cooled. No account is taken of process response to the release, for instance the pressure in the process system is assumed to be constant during any release. The rate of release is either calculated by the system itself or specified by the user as input data. The discharge may result in a BLEVE (Boiling Liquid Expanding Vapour Explosion), pool fire, jet fire, spray fire, flash fire, an explosion inside a building, an unconfined vapour cloud explosion (UVCE), or the spreading of toxic gases, or any combination of these.

The estimate of the consequences of an accidental release is based on well established models. The evaluation of a scenario can be characterised as a dialogue between the user and the computer. The system asks some questions and then runs a small calculation program after the answers have been provided. Depending on the result, new questions can be asked and so on.

Several calculation programs are included in the accidental release part of the system. A brief reference to the various models used in these programs is presented below, while an indepth description is presented in Appendix A.

The release rate calculation is based on the models in [Guidelines for Chemical Process Quantitative Risk Analysis (CPQRA), 1989] for single phase and the methods in [Fauske and Epstein, 1987] for two-phase releases. For calculation of the concentration fields in the vicinity of the release, the method of [Chen and Rodi, 1980] is used. The calculation of the evaporation rate from a liquid pool is based on [Jensen, 1983] for those at a temperature below the ambient and a simplified model developed by US Air Force Engineering and Services Laboratory [Chems Plus, 1991] for pools at ambient temperature. Estimates of the concentration inside buildings is based on [Harris, 1983]. The program SLAB [Ermak, 1989] is used for the dispersion of gases outside buildings. As can be seen from above only well established models are used. What the system does, is basically to help the user by providing these models, with the appropriate

data, according to the scenario being evaluated and the output from the previous evaluation step.

The calculation of the effect of a jet flame on the surroundings is based on work by [Hawthorne, Weddell and Hottel, 1949], which can calculate the jet length of a gaseous release and [CPQRA, 1989] for the jet length of condensed gases. In addition, the information in [Räddningsverket, 1989] is used to calculate the radiation flux which causes severe burns and the model in [Whazan User's Guide, 1988] is used for the calculation of the radiation from a jet flame. For large pool fires the [Mudan and Groce, 1995] model is used, which takes into account the flame tilt due to the wind, when estimating the radiation. The radiation from a flash fire is estimated according to [Lees, 1980]. For unconfined vapour cloud explosions (UVCE), the TNT equivalent model is used [CPQRA, 1989]. For explosions inside buildings the Cubbage and Simmond model is used [Harris, 1983]. An estimate of the effect of a catastrophic tank failure and a BLEVE is undertaken according to [CPQRA, 1989].

The main difference between this expert system and other consequence analysis programs, is that when using these, one has to be very familiar with the modelling of the accidental release, since no warnings are given, when one is outside of the validation limits of the models used. In this expert system warnings are given and the system also provides an estimate of the properties that are currently being calculated. In addition, this program takes releases within a building into consideration, but it does not evaluate the concentration fields inside a building, when the release occurs outside. Estimating damage to a component is also a feature which other programs do not contain.

## 2.4 Effect of heat on components

Estimating the thermal effects that a fire environment can have on a specific component is a rather difficult task. Some of the reasons for this are:

- experimental data on damage criteria for components of various types, sizes and shapes is limited.
- such criteria, when determined experimentally, can be presented as a specific surface temperature, average component temperature, high temperature at a certain position inside or on the surface of the

component. Others include the duration of a certain heat irradiation and the duration of a specific surrounding temperature.

- the above must be compared to a real fire environment, where a component is subjected to time varying radiation and convective heat transfer (from either flames or the gas layer).
- certain local effects cannot in practice be modelled.
- heat transfer to and within the component usually requires complex models, due to complicated geometries, presence of cavities, the number of materials involved, etc.

Classical heat transfer provides simple expressions which allow calculation of the surface temperature of an object which is subjected to a given thermal load. However, by using such simple expressions the component must be assumed to be either a "lumped mass" of a certain size, or "semi-infinite". Furthermore, the component must be relatively homogeneous and have known thermal properties ( $k\Delta c$ ). This is rarely the case for the components considered here and therefore FREIA does not attempt to calculate component surface temperatures.

It is therefore obvious that certain empirical procedures, in conjunction with engineering judgements, must be followed in order to estimate whether a component will fail when subjected to a given fire environment. The following section outlines a simplified methodology for this purpose.

### 2.4.1 Damage criteria

The damage criteria concept used in FREIA can be expressed graphically as shown in figure 2.2.

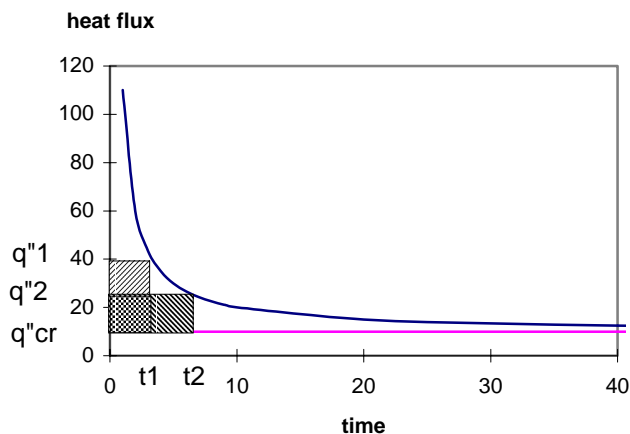


Figure 2.2. The principles behind the damage criteria concept in FREIA

A component can be considered to withstand a high heat flux ( $q''_1$ ) for a short time ( $t_1$ ), a somewhat lower flux ( $q''_2$ ) for a longer time ( $t_2$ ) and a relatively low heat flux ( $q''_{cr}$ ) for a very long time (infinite). Here, it is assumed that the component can withstand a certain dose of heat flux and after [Frank and Moieni, 1986] eq. 2.2 can be used

$$(q''_1 - q''_{cr}) t_1 = (q''_2 - q''_{cr}) t_2 = E_{cr} \quad (2.2)$$

In other words, it is assumed that the shaded areas in figure 2.2 are of equal size. Here,  $E_{cr}$  is the maximum heat dose which the component is assumed to withstand. FREIA therefore only requires the user to supply data on component damage criteria consisting of:

- a) a certain level of heat flux which the component can withstand for a long time ( $q''_{cr}$ )
- b) a certain level of heat flux which the component can withstand for a certain specified length of time ( $q''_1$  for  $t_1$  or  $q''_2$  for  $t_2$ ).

For certain types of components there exists some data which can be used directly. In other instances there may exist data where the component has been subjected to elevated temperature for a certain length of time, this data can be approximately transformed to the above format. Where there is no data available the user must specify criteria which he considers to be on the safe side.

#### 2.4.2 Calculation of heat received by a component

In order to estimate the heat flux received by the component, the user must specify its position and also that of the fire. The user can specify two types of component positions; a component situated at a certain point, or a component whose position is defined by a line (for example a pipe or a cable). In the latter case the component position is transformed to a point where the view factor from the flame is a maximum.

FREIA assumes that the component can be subjected to heat from four sources:

- radiation from the hot gas layer

- radiation from the flame
- convective and radiative heat transfer due to direct contact with the hot gas layer
- convective and radiative heat due to direct contact with the flame

It is further assumed that if the component is surrounded by the hot gas layer then it is shielded from the flame's radiation.

The magnitude of the heat flux from one object to another is a function of the temperature difference between the two objects. In our case, as mentioned above, no attempt is made to calculate the surface temperature of the component. The following expressions therefore conservatively assume that the object's surface temperature  $T_0$  is ambient throughout the calculations.

#### Radiation from the hot gas layer

The hot gas layer is assumed to be a plane sheet with surface temperature  $T_g$  (output from FIRE SIMULATOR) at a certain height above the component. The heat flux from the hot gas layer to the component  $\dot{q}_g''$  is written as

$$\dot{q}_g'' = (T_g^4 - T_0^4)\sigma\epsilon F_g B \quad (2.3)$$

where  $\Phi$  is the Stefan Boltzmann constant ( $5.67 \cdot 10^{-8} \text{ W/m}^2\text{K}^4$ ),  $\epsilon$  is the gas layer emissivity (assumed to be 0.8) and  $F_g$  is the view factor from the gas layer to the component.

The view factor is calculated in a classical manner, using the equations for plane surfaces, as well as using the additive and subtractive properties of the view factor equations. In order to do this, FREIA utilises information on the length and width of the room and also the components position in it. In addition, the height of the smoke layer (from FIRE SIMULATOR output) is used to calculate the relative distance between the component and the underside of the gas layer. Thus both the hot layer gas temperature and the view factor change with time.

#### Radiation from flame

The flame is assumed to have a cylindrical shape with a certain diameter and length (calculated in FIRE SIMULATOR) and be positioned at a certain distance from the component. The heat flux from the flame  $\dot{q}_f''$  is written as

$$\dot{q}_f'' = (T_f^4 - T_0^4)\sigma\epsilon F_f C \quad (2.4)$$

where  $\epsilon$ , the flame emissivity is assumed to equal 0.8,  $F_f$  is the view factor from the flame to the component and  $T_f$ , the flame temperature is assumed to be 1100 K.

The view factor is calculated using the equations for cylinders [Siegel and Howell, 1981], as well as, using the additive and subtractive properties of the view factor equations. FREIA utilises information on the flame length and diameter and the components position relative to the flame. The fire diameter can increase with time and the component may suddenly be engulfed in the flames. In this case, the heat flux is calculated as in the "direct contact" case below, but using a constant flame temperature of 1100 K.

#### Heat transfer due to direct contact with the hot gas layer or flame

Once the hot gas layer has descended to the component, the above radiative heat transfer from the flame and the gas layer is assumed to cease. The component is then assumed to be subjected only to the radiative and convective heat flux due to direct contact with the hot gas layer.

However, the radiative heat flux from the flame and the gas layer, as calculated by equations (2.3) and (2.4), cannot be directly compared with the heat received from a surrounding hot gas mass. In order to compare the two types of heat transfer, the effect of the hot gas mass must be expressed as a heat flux to the component. As mentioned earlier the main approximation is that  $T_s = T_0$ . There is some justification for such an approximation since the gas temperature is often relatively low. The following engineering assumptions are made, in order to achieve an analytical solution of the general heat conduction equation [Carslaw and Jaeger, 1959]:

The heat flux from the gas mass  $\dot{q}_{gm}''$  is written as

$$\dot{q}_{gm}'' = (h_r + h_c) (T_g - T_0) D \quad (2.5)$$

where  $h_c$  is the convective heat transfer coefficient (assumed here to be  $20 \text{ W/m}^2 \text{ K}$ ) and  $h_r$  is the radiative heat transfer coefficient, written as

$$h_r = \sigma \epsilon (T_g^4 - T_0^4) / (T_g - T_0) E \quad (2.6)$$

The emissivity of the gas layer  $\epsilon$  is again assumed to be 0.8.

### Total heat flux received by the component

When the component is immersed in the hot gas layer then  $\dot{q}_f''$  and  $\dot{q}_g''$  are assumed to be zero. If this is not the case, then  $\dot{q}_{gm}''$  is assumed to be zero. The total heat flux received by the component at each time stage is simply calculated from

$$\dot{q}_{tot}'' = \dot{q}_f'' + \dot{q}_g'' + \dot{q}_{gm}'' F \quad (2.7)$$

### Comparing damage criteria with the heat flux received

The shaded areas in figure 2.2 shows the heat dose which the component is assumed to withstand, while an example of the heat flux received by a component, with  $\dot{q}_{tot}''$  (from equation (2.7)) plotted against time, is shown as figure 2.3.

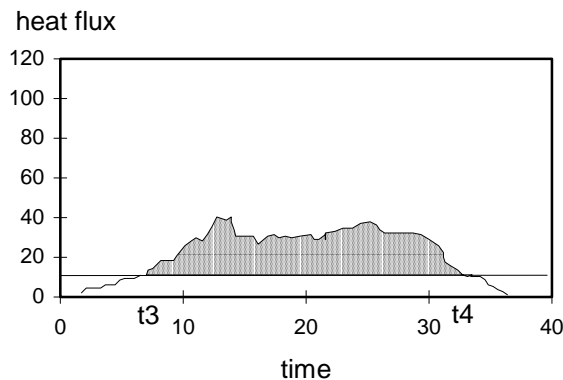


Figure 2.3. Example of heat dose received by a component.

By integrating over the shaded area the total dose received  $E_r$ , can be compared to the critical heat dose,  $E_{cr}$  (as calculated from equation (2.2)). The dose received is thus calculated from

$$E_r = \int_{t_3}^{t_d} (\dot{q}_{tot}'' - \dot{q}_{cr}'') dt G \quad (2.8)$$

Furthermore, the time to damage  $t_d$  can be calculated by solving  $t_d$  using the equation

$$E_{cr} = \int_{t_3}^{t_d} (\dot{q}_{tot}'' - \dot{q}_{cr}'') dt H \quad (2.9)$$

since  $E_{cr}$  is known from equation (2.1).

### 2.4.3 Calculation of damage criteria

The damage to a component is often considered to take place then the component reaches a certain temperature either at the surface or inside. In FREIA the damage criteria is expressed as a heat flux dose. The above critical temperatures must therefore be transformed into heat flux doses. The following four types of components have been identified as important when evaluating damage in industry:

- semi-infinite solid, critical temperature is at surface;
- concentrated mass, critical temperature is average temperature of component;
- component within a cabinet;
- pipe with flowing gas or liquid.

#### The semi-infinite solid

The surface temperature  $T_s$  of a semi-infinite solid subject to a constant heat flux  $\dot{q}''$  is calculated from

$$T_s - T_0 = \frac{\dot{q}''}{h_{eff}} \left( 1 - e^{h_{eff}^2 t / (k\rho c)} \operatorname{erfc} \sqrt{h_{eff}^2 t / (k\rho c)} \right) \quad (2.10)$$

where  $T_0$  is the initial temperature,  $kc$  is the thermal conductivity, density and specific heat of the material and  $t$  is the time. The heat transfer coefficient  $h_{\text{eff}}$  is given by

$$h_{\text{eff}} = h_c + \frac{\sigma(T_s^4 - T_0^4)}{T_s - T_0} \quad (2.11)$$

where  $h_c$  is the convective heat transfer. By knowing the critical surface temperature and choosing a time, or a heat flux, the heat flux or time required to reach the critical temperature can be calculated.

### The concentrated mass - "lumped heat capacity"

When the heat conduction within the material is much higher than the heat transfer across the surface, the component can be treated assuming a "lumped heat capacity", i.e. when

$$\frac{h \cdot (V / a_s)}{k} \leq 0.1 \quad (2.12)$$

where  $V$  is the volume of the component and  $a_s$  is the surface area of the component subject to heating. The temperature increase of the component  $T$ , subject to a constant radiation is then given by

$$\Delta T_{n\Delta t} = \sum_{i=1}^n \frac{\Delta t \cdot a_s}{mc} (\dot{q}'' - h_{\text{eff}}(T_{i-1} - T_a)) \quad (2.13)$$

where  $m$  is the mass of the component and  $t$  is a time step. By choosing a heat flux it is possible to calculate the time required for the component to exceed the critical temperature.

### The component within a cabinet

The component is considered either to be placed, with thermal contact, on the wall of a cabinet, or without thermal contact on the floor. The temperature increase of the cabinet wall as a function of time assuming that the wall is thin is given by

$$\Delta T_{n\Delta t} = \sum_{i=1}^n \frac{\Delta t \cdot a_s}{mc} (\dot{q}'' - 2h_{\text{eff}}(T_{i-1} - T_a)) \quad (2.14)$$

For the case when the component is placed on the wall of the cabinet, its temperature is assumed to equal that of the wall. When the component is placed on the floor, the heating of the component is assumed to be due to radiation from the cabinet wall, this is given by

$$\dot{q}''(i\Delta t) = \sigma(T_w^4 - T_{\text{comp}}^4) \quad (2.15)$$

where  $T_w$  increases with time according to eq. (2.14). The temperature increase of the component is then given by

$$\Delta T_{\text{comp}}(n\Delta t) = \sum_{i=1}^n \frac{\Delta t \cdot a_s}{mc} (\dot{q}''(i\Delta t) - h_c(T_{\text{comp}}(i-1) - T_a)) \quad (2.16)$$

Here it is assumed that the view factor between the cabinet and the component equals 1, the heating of the air within the container is not included in the calculations. By choosing a heat flux and then iterating, the time to damage can be calculated.

### Pipe with flowing gas or liquid

The damage criteria for a pipe containing a flowing gas or liquid is calculated using the program HSLAB.

## 2.5 Other effects of fires and accidental releases on humans, components and the environment

Estimating factors other than the effect of heat on components is difficult and if even considered in FREIA only crude methods are used. Some of these additional factors are discussed below.

### 2.5.1 Corrosive effects

No advice is provided by FREIA on what concentration levels and substances which can cause corrosive damage.

In estimating the corrosive effect on components using FREIA, it is possible to calculate the concentration inside the building, due to an accidental release, and for how long time it exceeds a certain value. For external discharge a concentration profile is calculated. From this profile the radius within which the concentration exceeds a specified level for a specified time is calculated.

In the fire evaluation chain no calculation is undertaken as to which gases are produced, except for excess fuel and CO. The CO is estimated assuming a certain fraction of the fuel forms CO. Some extinguishing agents produce corrosive gases, these are not calculated by FREIA.

### 2.5.2 Toxic effects

Estimation of possible toxic problems by FREIA is undertaken using the same rather basic approach as that used for corrosive effects.

However, it is possible to estimate a toxic dose in the same manner as the heat dose. This toxic dose can then be used in the probit function to estimate the percentage of people affected, or killed, in the area covered by the toxic substance [CPQRA, 1989]. This is not however implemented in FREIA, but will be discussed further in chapter 5.

The toxic dose is given by

$$\int_{t_0}^{t_{\text{end}}} C^n dt \quad (2.17)$$

where the exponent  $n$  ranges between 0.6 and 3 and  $C$  is the concentration. By setting  $n$  to 1 and subtracting a critical level, the expression becomes

similar to the heat dose function used for estimating damage to components.

### 2.5.3 Environmental effects

Estimating environmental effects is a complex field. In FREIA the only aid is the calculation of the concentration profile outside the building due to an accidental release. No calculation of material deposited on the ground, trees, etc. is carried out.

### 2.5.4 Human burns

Burns on bare skin are assumed to require the radiation doses taken from Table 2.1 below. The radiation from a jet flame is calculated assuming that it consists of five point radiation sources of equal magnitude, and equally distanced over the flame length. Humans are assumed to remain in the vicinity of the jet flame for 10 s. The radiation from a pool fire is calculated using the view factor of a tilting cylinder. The radiation from a flash fire is calculated using the five point radiation sources approximation. The cloud is assumed to be elliptical and to expand by a factor of 8 (conservative assumption) upon ignition. The estimate of the duration of the flash fire is based on radiative cooling of the cloud. The radiation from a BLEVE is assumed to emerge from a point source.

Table 2.1 Radiation dosages required to burn exposed skin.

Burns	Radiation dose (kJ/m <sup>2</sup> )	
	1 s duration	10 s duration
1 <sup>st</sup> degree	50	80
2 <sup>nd</sup> degree	120	200
3 <sup>rd</sup> degree	200	350

### 2.5.5 Pressure effects

For estimating the pressure effects of explosions due to accidental releases the various distances at which specified pressures develop are calculated. This calculation is based on the TNT-equivalent model. This is further discussed in Appendix A.

## 2.6 Auxiliary databases

Included in the FREIA package are some auxiliary databases to help the user in supplying FREIA with appropriate input data. In Appendix B the auxiliary databases are described.

## 2.7 An example of a calculation performed with the aid of FREIA

An example of the outcome from calculations performed using FREIA on the case study illustrated in figure 2.4 is given below. This consisted of a room 18x24x4.5 m, with smoke ventilation in the ceiling 4x1m<sup>2</sup> and a detector which activates at 70°C. The room has a row of windows, 1.5 m high, close to the ceiling along one of the long walls and one row 9 m long and 1.5 m high on each of the short sides close to the ceiling. There are two small doors in the room 2.1 m by 1 m and one large door 4 x 3 m.

The room contains the following components:

- An engine weighing 1500 kg which can withstand an ambient temperature of 60°C and a maximum internal temperature of 80°C.
- A pump weighing 470 kg which can withstand an ambient temperature of 60°C and a maximum inner temperature of 100°C.
- Welding equipment with acetylene gas that can withstand 50°C ambient temperature for an infinite time and 500°C for 10 minutes.
- 3 cabinets with electrical equipment that can withstand 55°C as the ambient temperature.
- cables.

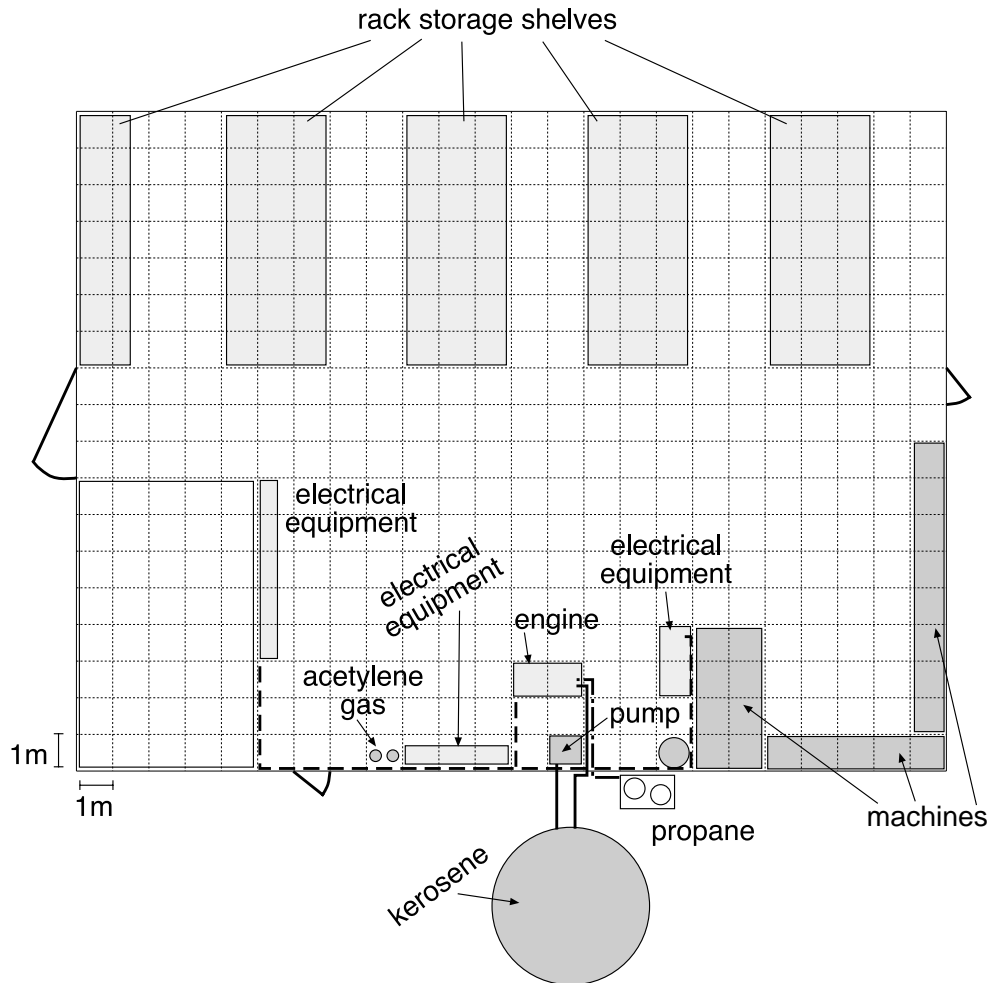


Figure 2.4 Schematic diagram of room used in case study.

The temperature levels for the acetylene gas cylinder are recalculated into an equivalent heat flux to obtain the damage criteria. The damage criteria for the pump and engine are calculated using a "lumped heat capacity" and by assuming that half the total surface area is exposed to radiation. The damage criteria for the cables are taken from [Frank and Moieni, 1986]. The room also contains a propane pipe with a discharge capacity of 0.065 kg/s. In addition, there are pipes containing kerosene and some rack storage shelves. As possible fire scenarios a propane jet fire, a kerosene spray fire, a kerosene pool fire, a cable fire and two different fires in the rack storage shelves were chosen. These six scenarios are combined with 6 different ventilation situations. The ventilation conditions used were as follows: one small door open, the large door open, all openings closed, small door and roof ventilation open, large door and roof ventilation open and finally, with only roof ventilation.

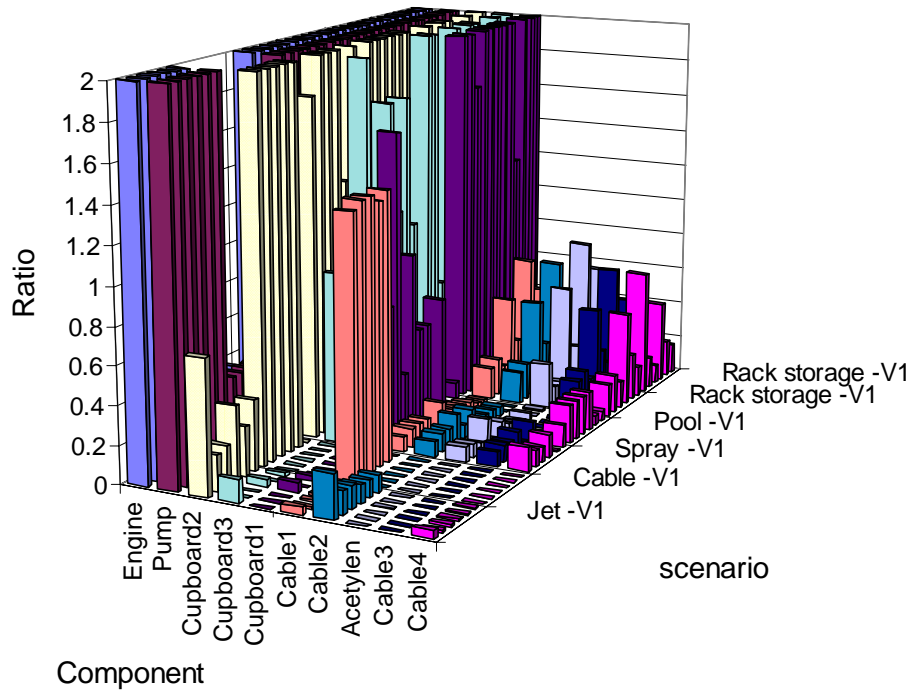


Figure 2.5 Relation between incident heat flux and damage criteria.

The results of these calculations are presented in figure 2.5. All scenarios where the ratio is 1 or more indicates that a component is damaged. As can be observed from the figure ventilation has little effect on number of damaged components in this case study. However, the spray fire, the pool fire and the fires in the rack storage shelves could not be allowed to occur, if it is essential for normal production to be promptly established after any incident. For example the engine, the pump and one of the cupboards are damaged, in almost all of the scenarios and therefore more fire protection is required.

## 2.8 Weak links in the evaluation

FREIA has been found to be a valuable tool for exposing weak points when it comes to fire safety. However, during the development and use of FREIA some weak links in the evaluation chain have been identified.

The spread of fire is an area where considerable research still remains to be undertaken, this will not however be discussed further in the present thesis.

The precise evaluation of when a detector is activated is very important in the estimation of the damage caused by a fire. It is possible to calculate when a heat detector, such as a sprinkler is activated for simple geometries using FIRE SIMULATOR. Smoke detectors can be treated similarly, i.e. they are assumed to behave like a heat detector with a low RTI value. However, it is not possible to use FIRE SIMULATOR, if the ceiling slopes, or if there are beams in the ceiling, etc. It is also rather questionable to assume that a smoke detector acts as a heat detector. The problems with evaluating detector activation are discussed further in Chapter 3.

Extinguishing systems are important in keeping any fire damage to as low a level as possible. In FREIA the fire is supposed to be extinguished immediately on activation of the extinguishing system. However, fires are not often completely extinguished by the extinguishing system. Sprinklers, for instance, are usually only designed to limit the fire. Some halon replacement agents can even increase the fire if not designed correctly. These problems are discussed in Chapter 4.

The repercussions of fires and accidental releases on humans, components and the environment is an area where little is known. This will be discussed further in Chapter 5.

## **3 Smoke and Heat Detection**

In industry, there is usually some kind of detection system present to initiate the release of extinguishing media and/or send an alarm to the fire brigade. These detectors can detect heat, particulate matter or radiation from the flame. Heat and smoke detectors are the most common. The time elapsing from the start of the fire to detector activation depends on the detector and the fire scenario. This includes the fuel, the rate of growth, whether it is a flaming or smouldering combustion, the type and location of the detector and the air flow pattern in the room before the fire starts. The ventilation, beams in the ceiling, porous suspended or false ceilings, other heat sources, can for instance considerably delay the time to detection.

Presently, the prescriptive rules and advice for the placement of detectors, include the impact of the above mentioned complications to only a very limited extent [RUS 110, NFPA 72]. One possible approach to develop better rules and advice is to undertake experiments. However, such investigations are time consuming and expensive, and it is also difficult to include all possible scenarios and detector systems. At the present time the development of fire codes is towards performance based design, this often requires computer modelling of detector activation. Two types of computer modelling are available today, i.e. two-zone models and Computational Fluid Dynamics (CFD). However, two-zone models such as FIRE SIMULATOR do not include the various effects described above, instead CFD models must be used. For heat detectors it is a rather straight forward problem to calculate the time to detection using CFD-models. For smoke detectors the problem is much more complicated.

### **3.1 Heat detectors**

There are basically two types of heat detectors available, those which send out an alarm signal when the surrounding temperature has reached a certain value, and those which send out an alarm signal when the rate of temperature rise exceeds a certain value. Those which are activated at a certain temperature usually consist of a fusible link, a bimetallic thermometer, or a glass bulb containing a liquid which starts to boil at a specific temperature which then cracks the glass bulb. The rate of rise detectors usually consist of two thermistors, one placed in the open so that it rapidly responds to the heat from the fire and one placed in a protected

place, whether to give alarm is determined from the voltage difference between these thermistors.

The fact that the gas temperature reaches the activation temperature does not activate the detector instantaneously due to the thermal inertia of the detector. The thermal inertia is usually expressed as an RTI-value (Response Time Index), of dimensions  $m^{1/2}s^{1/2}$ , which is suitable for use in simulations. The RTI-value is easily determined experimentally. Even better modelling is achieved, if a conduction term  $C$  (units  $W/^\circ C$ ) for the conduction losses from the detector, is included. In addition, once the sensing element has reached the activation temperature the fusible link has to melt and the liquid has to boil and crack the bulb. An actuation term  $CHP$  ( $^\circ C$ ) should therefore be included [Ingason, 1996].

### 3.2 Smoke detectors

There are basically two types of smoke detectors in use today, ionisation or optical. In ionisation detectors the air is ionised with the aid of a small radioactive source. The ionised air molecules are attracted by two electrodes and thus a small current develops. When smoke is also present the smoke particles and the ionised molecules are attracted to each other. This results in heavier ionised particles and since the electric force present is not strong enough, compared to the particles' inertia, they do not strike the electrodes and the current therefore decreases. Optical detectors consists of a light source and an optical detector, e.g. a photodiode, they either measure the extinction of the light in the forward direction, or else the scattered light.

Smoke detector response is dependent on the velocity of the smoke particles, their direction, the number of particles and the size of the particles. Ionisation detectors are more sensitive to small smoke particles ( $<0.1$  m), from open fires, while optical detectors are more sensitive to glowing fires, where the smoke particles are larger (1-10 m).

Present smoke detectors are becoming more and more sophisticated in order to minimise false alarms. The entry of smoke into the detector chamber is complex, also the development of the signal treatment is moving towards the use of fuzzy logic. This makes it difficult to develop mathematical models for smoke detector activation. Presently no model

exists for predicting whether or not a detector, subject to a certain flow of smoke, will be activated.

### 3.3 Influence of complex geometries, ventilation and heating sources

Complex geometries, such as sloped, porous, suspended and/or false ceilings can considerably delay the time to detector activation. Beams in the ceiling can also delay, or decrease the time to detector activation [Schneider and Könnicke, 1995; Davis, Forney and Bukowski, 1995].

A very rough estimate [Thomas, 1996] for the rate of heat release required for the fire to take control of the air flow pattern in the room, can be undertaken by comparing:

- the mass flow in the fire plume, with the mass flow extracted from the room by ventilation;
- the velocity in the fire plume, with typical velocities in the room;
- the temperature rise in the fire plume, with the temperature stratification;
- the rate of heat release due to the fire, with other heat sources.

The mass flow in a plume can be expressed as [Zukoski, Kubota and Cetegen, 1981]

$$\dot{m} = 0.071\dot{q}^{1/3}z^{5/3} \quad (3.1)$$

where  $\dot{q}$  is the rate of heat release in kW and  $z$  is the elevation above the fire source in metres. The velocity at the centreline of the plume is given by [Heskestad, 1984]

$$u_0 = 3.4[g / (c\rho_\infty T_\infty)]^{1/3} \dot{q}_c^{1/3} (z - z_0)^{-1/3} \quad (3.2)$$

where  $g$  is the acceleration of gravity,  $c$  is the specific heat of air,  $\rho_\infty$  is the ambient density,  $T_\infty$  is the ambient temperature,  $\dot{q}_c$  is the convective heat release rate (kW) and  $z_0$  is the elevation of the virtual origin above the fire source. The temperature at the centre axis of the plume is given by [Heskestad, 1984]

$$\Delta T_0 = 9.1[T_\infty / (gc^2\rho_\infty^2)]^{1/3} \dot{q}_c^{2/3} (z - z_0)^{-5/3} \quad (3.3)$$

where  $T_0$  is the temperature increase at the centreline of the plume.

Ventilation is often expressed as the number of air changes per hour. In a dwelling it is normal to have 3 air changes per hour. At a theatre where people often smoke, the ventilation rate is higher at perhaps 10 air changes per hour. In industry the ventilation rate is dependent on the type, however, a rough average could be 5 air changes per hour.

Air velocity in a dwelling is usually close to 0.3 m/s, if higher the indoor climate feels uncomfortable because of the draught. In a theatre the velocity can be a little higher at perhaps 0.5 m/s, while in industry the velocity can be about 1 m/s.

In normal rooms the temperature stratification is about 1°C/m, however, the stratification can be higher due to solar radiation, etc. In industry and theatres the stratification is usually higher at 2-3°C/m.

A comparison between the mass flow in the plume close to the ceiling calculated from equation 3.1 and the ventilated mass flow for a bedroom 3x3x3 m with a ventilation rate of 3 times per hour, means that the rate of heat release due to the fire would have to exceed 0.23 W in order to produce more smoke than is taken away by the ventilation. This comparison assumes that all air that is ventilated from the room is extracted through a ceiling vent. However, equation 3.1 is basically invalid for such a low rate of heat release as 0.23 W.

Comparing the velocity in the plume close to the ceiling with the normal velocity of 0.3 m/s in the same bedroom necessitates a rate of heat release greater than 44 W. In order for the maximum temperature in the plume to exceed the temperature increase close to the ceiling due to stratification of 1°C/m, the rate of heat release must exceed 60W in the room. A normal radiator has a power of about 1 kW; therefore the fire must release at least the same power in order to control the air stream pattern in the room.

Carrying out similar comparisons for a theatre (30 x 30 x 10 m), with a ventilation rate of 10 times per hour, would require a rate of heat release of at least 750 kW to produce more smoke than can be ventilated. In order for the plume velocity to be higher than the normal velocity in the theatre (0.5 m/s), the rate of heat release would have to be greater than 670 W. To overcome the effect of stratification of 3°C/m, the rate of heat release

would need to be in excess of 380 kW. To heat a theatre close to 30 kW is usually required, this could be provided by 10 radiators and therefore the fire would have to be at least 3 kW in order to be able to control the local air stream pattern.

For an industrial building (100 x 100 x 20 m) with a ventilation rate of 5 times per hour the same comparisons necessitate that, in order to produce enough smoke it would require 32 MW. For the velocity in the plume to be greater than a normal velocity in the building of 1 m/s, it would require 11 kW and to overcome the stratification of 3°C/m 6 MW would be required. Industrial machines and engines can produce 200 kW in excess heat and therefore, in order for the fire to take control of the air flow it would have to produce at least 200 kW.

The above comparisons of course are very crude. For the bedroom the comparison with the heating system places the highest demand on any fire, i.e. in excess of 1 kW. In the theatre and industry cases the toughest demand on the fire is the formation of enough smoke to overcome the ventilation, i.e. a rate of heat release in excess of 750 kW for the theatre and 32 MW for industrial buildings. Assuming that all air that is ventilated from the room, is taken at the ceiling level, just above the plume is of course not completely correct. However, the demand from the stratification comparisons is 380 kW and 6 MW respectively; this is probably not too conservative a requirement, since the stratification could be higher due to solar radiation and also it is the maximum temperature of the plume which is compared to the stratification temperature.

### 3.4 Performance based design

Instead of prescriptive rules several performance based fire codes have been recently developed [Committee draft ISO CD 13387; BBR94, 1995; "Fire Engineering Guidelines", 1996]. These require that the detectors produce a warning before the fire has reached a certain level. In order to investigate the designs which can fulfil this requirement, experiments can be conducted, or preferably the time to detector activation calculated. It is also essential to be able to calculate time to detector activation in risk and hazard analysis. There are basically two options available today to calculate detector activation, correlated expressions based on ceiling jet theory [Evans and Stroup, 1985; Cooper, 1988] or using CFD-models.

### 3.4.1 Ceiling jet theory

The ceiling jet theory assumes that the ceiling is smooth, has no vents or beams, is not sloping, is non-porous, and not suspended, or false. It only takes into consideration the height of the room. No account is taken of walls close to a detector. The temperature and velocity is radially symmetric with the fire plume in the centre. In addition, [Cooper, 1988] takes into account differences in temperature and velocity in the ceiling jet depending on the distance from the ceiling.

In FREIA, as in most two-zone models, the detector activation calculation is based on ceiling jet theory [Evans, 1984; Alpert, 1972]. Heat detector activation is calculated taking account of the heat detectors RTI-value. Smoke detector activation is calculated assuming that the smoke detector has a low RTI value and is activated at a certain temperature.

### 3.4.2 Computational Fluid Dynamics (CFD) modelling

There are several different CFD models available today, general purpose models such as PHOENICS, Flow3D, FLUENT, SHIVA and those developed for fire purposes, including JASMINE, SOFIE and SMAFS. All these models solve the conservation equations for mass, movement, energy and the species in each control volume of the room being evaluated. To solve these equations a turbulence model is required, usually a buoyancy modified k- $\epsilon$  model is used, and also a model for the combustion. For this the simple assumption is "mixed is burnt", this assumes that as soon as the fuel and oxygen are mixed it is burnt in a one step reaction.

In CFD calculations about 10 - 100 000 control volumes are used and it is also often possible to take advantage of symmetries in the room so that only a part of it needs to be simulated. The output from CFD-calculations, are for each control volume, the temperature, gas velocity, gas concentrations, pressure, etc. as a function of time.

CFD can model the effect of walls, beams and sloped, porous, false and/or suspended ceilings. In addition, it can take into account the ventilation and also additional heat sources. In Paper II a calculation of the air stream pattern in a bedroom with a radiator and a fire has been performed, using

the CFD-code JASMINE. The fire was assumed to increase linearly from 0 to 10 kW in 3 minutes. The simulation showed that the convective flow due to the fire was greater than the convective flow from the radiator, when the rate of heat release due to the fire was about 1.5 times higher than the power of the radiator.

It is possible to model heat detector activation with a reasonably good accuracy using CFD for most scenarios, i.e. the temperature and velocity fields are modelled with 30% accuracy. There are however problems which remain to be solved. The standard buoyancy-modified  $k-\epsilon$  turbulence model considerably under-predicts the width of the fire plume [Nam and Bill, 1994; Tuovinen, 1996]. Shadow effects of the frame of the detector are difficult to include; this can to some extent be overcome by testing the heat detectors with a gas flow in several directions and thus obtaining several RTI-values. However, it is much more difficult to model smoke detector activation as discussed below.

### 3.5 Modelling smoke detector activation using CFD

In order to model smoke detector activation the formation and transport of the smoke to the detector must be simulated. In addition, the response of the detector to a specific smoke flow should be modelled.

#### 3.5.1 Soot formation

Soot formation is a complex process [Bockhorn, 1994]. In combustion the fuel is first degraded into hydrocarbon radicals. These radicals react and either complete the oxidation process or, especially in fuel rich conditions, form small unsaturated hydrocarbons such as acetylene according to complex reaction schemes. Hydrocarbon radicals are then added to the unsaturated hydrocarbons forming aromatic rings. These aromatic rings grow mainly by the addition of acetylene. The large rings then coagulate forming primary soot particles. In addition, gas molecules are picked up for surface growth. The soot particles also agglomerate forming aggregates.

This general description of soot formation is of course very brief, as the chemical and physical processes involved are complex. It is however

possible to satisfactorily model the soot formation in several laminar premixed flames using the simple hydrocarbons  $\text{CH}_4$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_2$  and  $\text{C}_3\text{H}_8$  as the fuel. However, in fires the flames are turbulent, not usually premixed and the fuel is complex. In order to simulate turbulent diffusion flames the reaction schemes must be reduced considerably. The soot formation process must therefore be approximated to using much simpler models. These usually include a nucleation, a surface growth, a coagulation and an oxidation term. Since the models are approximate they usually contain parameters that should be "calibrated" utilising data from the fuel and fire scenario. The soot models can therefore not presently be used to predict smoke detector activation.

### Soot measuring techniques

In order to be able to model the soot formation, accurate measuring techniques are required to determine the soot volume fraction, density, particulate size and number concentration.

One technique is simply collecting the soot on a filter and then weighing it [Choi, Mulholland, Hamins and Kashiwagi, 1995]. This method is more suitably applied in the plume region than in the flame region due to the problems with disturbing the flame and measuring the sample volume at high temperatures. The soot density is obtained by determining the volume of the compacted particulate. If only a small amount of soot is collected by thermophoretic techniques it is also possible to study the sample using an electron microscope (transmission electron microscopy, TEM) [Faeth and Köylü, 1995]. These techniques are rather time consuming and not always possible to adapt to the fire situation.

Another technique for measuring the soot volume fraction is monitoring the temperature of a rapidly inserted thermocouple and comparing the result with that obtained from thermophoretic mass transfer theory [Mcenally, Köylü, Pfefferle and Rosner, 1997].

The most widely used techniques are those based on optical measurements. However, estimating soot volume fraction, density, particle size, etc. from light attenuation and scattering experiments is complex. Soot volume fraction measurements are usually performed using light attenuation and the calculations are based on the Rayleigh scattering approximation, i.e.

the particles are small compared to the wavelength and spherical so the scattering is negligible, and all light attenuation is then due to absorption. However, several different values for the soot refractive index have been reported [Smyth and Shaddix, 1996], resulting in an uncertainty by a factor of 2 in the calculation of the soot volume fraction. In addition, as previously discussed, soot agglomerates into large aggregates. These aggregates are not spherical and too large for the Rayleigh approximation to be valid. Instead the Rayleigh-Debye-Gans (RDG) fractal aggregate scattering interpretation should be used [Köylü, 1997]. The difference in calculated soot volume fraction using the Rayleigh approximation compared to the RDG interpretation is dependent on the wavelength of the light and the fuel. In the visible region the Rayleigh approximation over predicts the soot volume fraction by 15-90% [Köylü and Faeth, 1994].

When measuring both the absorption and scattering of the laser light in laboratory flames both the particle concentration and the size can be obtained [Santoro, Semerjian and Dobbins, 1983]. In these measurements the soot particle size is smaller than the laser wavelength. A pulsed laser is often used to obtain more accurate data.

Another optical method is dynamic light scattering [Scrivner, Taylor, Sorensen and Merklin, 1986]. With this method the size distribution of the soot is calculated from the Doppler shift of the scattered light due to the Brownian motion of the particles.

Other laser based methods for measuring the soot volume fraction in flames include laser-induced fluorescence (LIF) from  $C_2$  in laser vaporised soot, and more recently laser induced incandescence (LII) [Bengtsson and Aldén, 1995].

### 3.5.2 Modelling the transport of the smoke

As previously discussed there is currently no satisfactory soot model available for the CFD codes. Several models are, however under development that will be valuable in the future for prediction of smoke detector activation, especially since they can calculate the size distribution, as well as, quantity of soot. For the present simpler approaches must still be used, such as assuming that the soot field closely relates to that of the temperature [Schneider and Könnicke, 1995; Davies et. al. 1995;

Tuovinen, Holmstedt and Bengtsson, 1996], or one of the compound concentration fields ( $O_2$ ,  $CO_2$  or  $CO$ ).

In Europe smoke detectors are tested according to EN54 [EN54] using six different test fires. During these tests the temperature, the smoke density and the ionisation current close to the detector are measured. The activation of the detector is tested and depending on the initial response to the above, the device is categorised into one of three classes A, B or C. The smoke density is measured using IR-radiation at a wavelength of 860 nm.

In Paper II the assumption is made that the soot concentration and smoke obscuration is closely related to the oxygen concentration. This assumption results in good agreement between the calculations performed using JASMINE and experiments conducted at Delta Electronics in Denmark according to the EN54 test standard for specific fires. However, for other fires the difference was found to be by as much as a factor of three.

Light attenuation and extinction in smoke are dependent on the wavelength of the light, the number concentration of soot particles and their size. Traditionally, in the "fire world", the smoke production is determined using a white light source or a HeNe-laser, 633 nm. Light attenuation according to the EN54 standard is measured using infrared light at a wavelength of 860 nm. In Paper II the smoke production from the EN54 test fires was determined using an incandescent lamp, operating at a colour temperature of 2900 K and a detector with the CIE photopic response curve according to the "room-corner" test in the Nordtest standard [NT FIRE 025]. The smoke production data was then used as input for the CFD simulations. The difference in wavelength between the EN54 standard and the smoke production experiments could to some extent explain the differences observed between the simulations and experimental results.

Several authors have, as expected, reported large differences in light attenuation which are dependent on the wavelength of the light [Tewarsson, 1988]. In addition, measurements using a tungsten lamp, a monochromator and a CCD-array [Andersson and Holmstedt, 1995] have shown that the slope of the normalised optical density, as a function of wavelength, varied with the rate of heat release (RHR). The measurements were performed at wavelengths between 590 and 890 nm in a duct above a fire, where all smoke was collected. The result from such experimental

investigations are presented in figure 3.1. The rate of heat release from the fire in this study is presented in figure 3.2. As observed, the RHR increased a factor of 7 between 180 and 300 s. From the smoke studies it was found that a higher smoke obscuration is related to a decrease in the slope of the obscuration-wavelength curve, indicating smoke agglomeration, see figure 3.1.

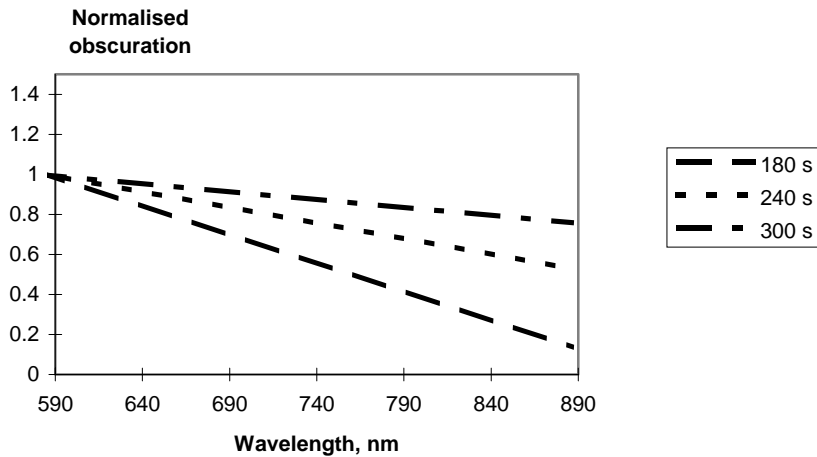


Figure 3.1 Normalised obscuration as a function of wavelength for different times of the TF1 fire according to EN54.

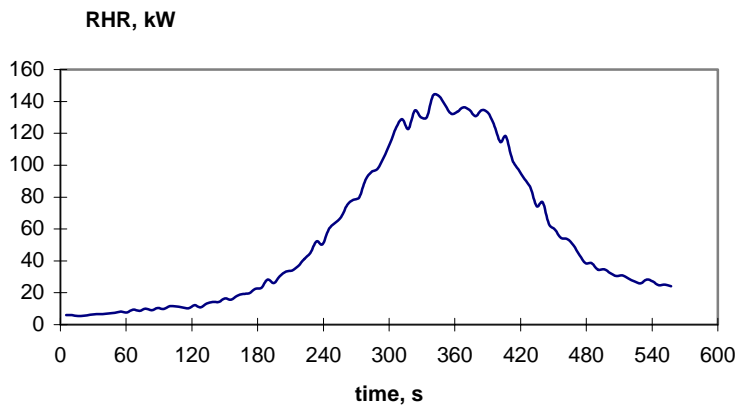


Figure 3.2 Rate of Heat Release for TF1 fire according to EN54.

It is not possible to completely justify the assumption that the oxygen and soot concentration correlates closely based on the results in Paper II due to the wavelength dependence problem. However, in Paper III the results from experiments measuring the soot concentration, as well as, temperature, velocity, oxygen, CO and CO<sub>2</sub> concentration profiles in the

plume above the flame are presented. A typical set of results are shown in figures 3.3 and 3.4 below. In these investigations good agreement was found between the various profiles, and no dip in the soot concentration was found at the centre of the plume. A dip in soot concentration in the flame has however been observed by [Coppalle and Joyeux, 1994].

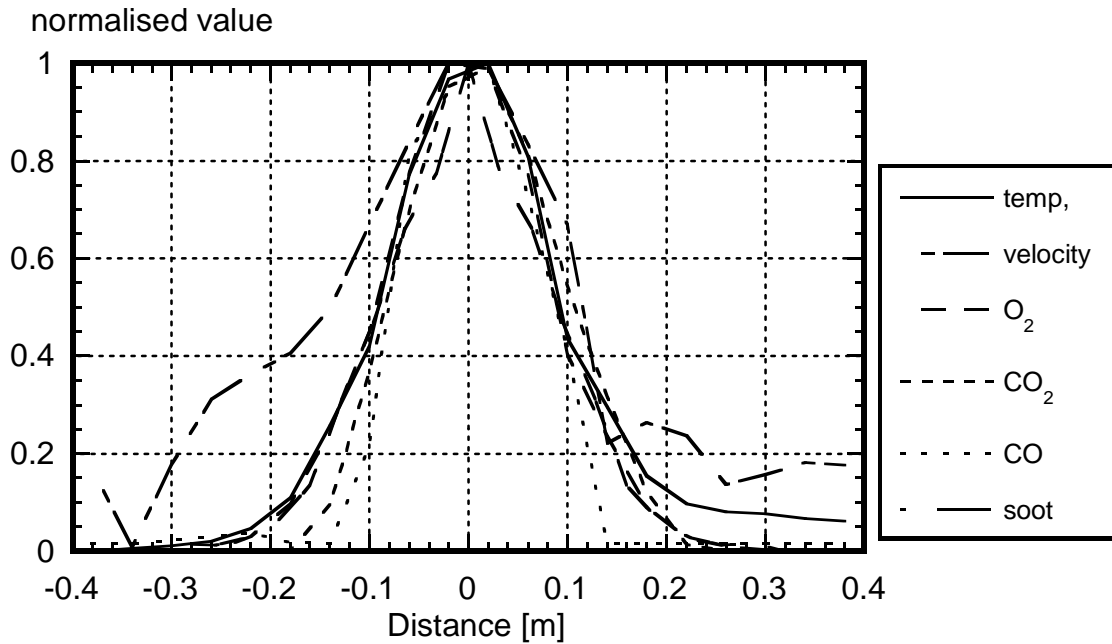


Figure 3.3 Normalised soot, CO<sub>2</sub>, CO, O<sub>2</sub>, temperature and velocity 0.9 m above a burner. The fire source is a 13 kW propylene diffusion flame.

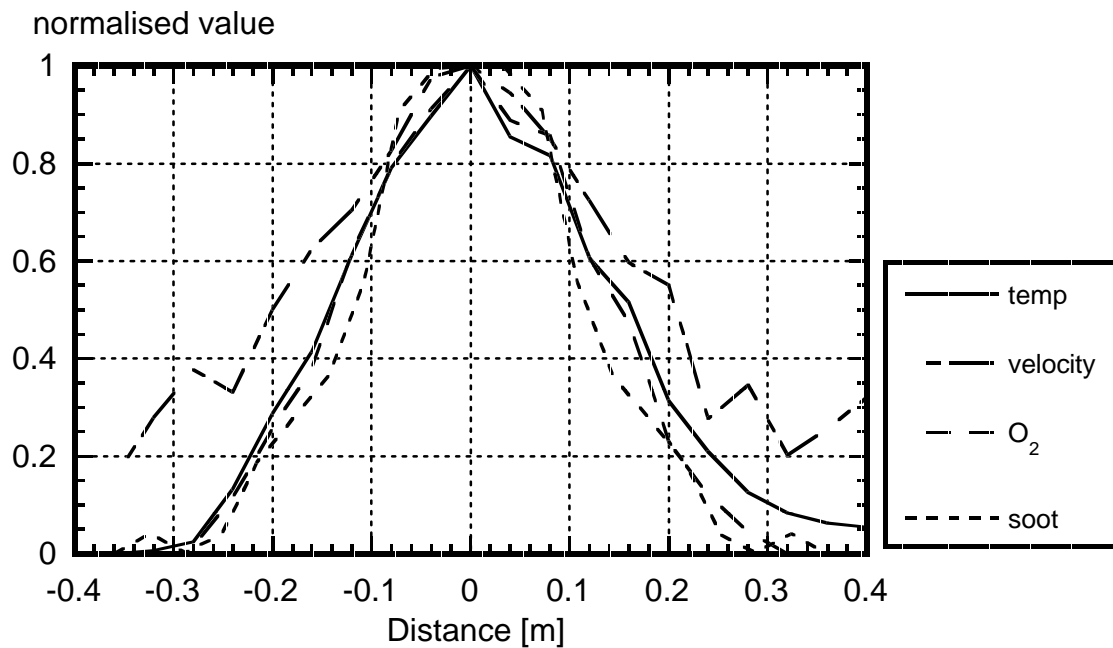


Figure 3.4 Normalised soot, O<sub>2</sub>, temperature and velocity 1.5 m above a burner. The fire is a 13 kW propylene diffusion flame.

It would appear from the above results that it is possible to model the soot volume fraction by assuming that the soot closely follows one of the compound concentration fields, it is probably preferable to couple it to the CO concentration since the CO and soot formation are to some extent mechanistically interrelated. However, as discussed in Paper III, as well as by several other authors [Nam and Bill, 1993; Tuovinen 1996], the standard buoyancy modified  $k-\epsilon$  turbulence model produces a far too narrow plume. This problem must be solved before a satisfactory simulation of the soot volume fraction can be obtained. The soot can also be introduced as an "inert gas" as proposed in Paper III, the quantity soot formed can then be either experimentally determined or chosen from published values. However, precautions must be considered when comparing the simulated with the experimental soot volume fraction. As discussed in Paper III the calculation of the soot volume fraction from light attenuation experiments is usually based on Rayleigh theory. The Rayleigh scattering approximation is not, however, valid for the large soot aggregates, instead the Rayleigh-Debye-Gans approximation should be used. In addition, there are several different refractive indexes reported for soot, which considerably increases the uncertainty of soot measurements.

### 3.5.3 Modelling the smoke detector response

In contrast to thermal detectors the response characteristics of smoke detectors varies widely depending on for instance the particle size distribution and the ionisation of smoke particles. There is no presently available model that can predict whether or not a detector subject to a specific flow and soot concentration will be activated. Heskestad [Heskestad, 1977] has introduced a simplified approach using the "characteristic length" of a detector, as a measure of the time lag required for the soot to reach the sensing element. VTT [Tuomisaari, 1996] have invented a method to determine this characteristic length.

Another approach is to take advantage of the fact that detectors are classified as A, B or C types in Europe depending on the smoke obscuration at which the detector is activated. It appears possible to simulate the smoke obscuration with CFD assuming that the soot concentration correlates with one of the compound concentration fields as proposed in Paper II. If there was a agreement between the wavelength used for both fire and detector calibration, there should be a considerable improvement in the simulations.

## 3.6 Concluding remarks

Problems remain to be solved before satisfactory modelling of detector activation can be accomplished.

The models for smoke and soot formation in a fire for use in CFD-models must be improved. Models exists for some fuels, these must however be calibrated experimentally.

The standard buoyancy modified  $k-\epsilon$  turbulence model often used in CFD-models, under-predicts the plume width considerably. This problem must be solved before an accurate modelling of smoke and heat detector activation can be accomplished. Work is continuing in this area and a new turbulence model was in fact used for the simulations performed in Paper III.

It is possible to estimate the soot volume fraction, or the smoke attenuation, using CFD simulation by adding the soot produced as an "inert

gas", or by assuming that the soot profile closely is comparable to one of the compound fields. There are however large uncertainties involved in transforming light attenuation measurements into soot volume fraction, or when transposing them into measurements using another wavelength. These transformations become even more uncertain, since so little is known about important smoke characteristics such as, ageing and the growth of soot aggregates.

There is currently no model available to estimate whether a smoke detector subject to a certain flow of soot is activated or not. When it comes to heat detectors the situation is much better. There are, however, some problems with shadow effects that remains to be solved.

## 4 Extinguishment

Some fires are developing so fast that they can cause severe damage before the fire brigade arrives to extinguish the fire. One way to prevent and mitigate damage due to such fires is using fixed extinguishing systems. Presently there are several different extinguishing agents available for use in industry, these include gas, liquid and solid phase agents. Some extinguish the fires completely, while others only slow down the rate of heat release. Some systems are total flooding or explosion suppression systems, while others are used for streaming/local application. All these systems are designed according to fire codes or the manufacturers instructions.

Some extinguishing agents are being phased out for environmental reasons. The replacement of these often requires performance based design. There is however no presently available models which can predict whether an extinguishing system extinguishes a fire, limits it or leaves it unaffected.

### 4.1 Different extinguishing agents used

A short description of the different extinguishing agents used, together with their advantages and disadvantages are summarised below. Some comments on design are also included.

#### 4.1.1 Gas phase extinguishing agents

Gas-phase agents are those with a normal boiling point below 20°C. Such agents used include halons, carbon dioxide (CO<sub>2</sub>) and inert gases, such as nitrogen and mixtures containing argon. One important advantage of gaseous agents is that no cleaning is required after a release of the agent in the absence of a fire, a couple of minutes of venting is all that is required. However, gaseous systems except halons require rather a large storage area, especially nitrogen and argon mixtures since they are stored as compressed gases. For all these agents, except the halons, the inerting concentration is so high that it is difficult to distribute the gases into the

room in a sufficiently short time, without breaking walls and windows due to the consequent pressure increase.

### Halons (Halon 1211 and Halon 1301)

Probably the most common agents used until recently are halons (i.e. Halon 1301 and Halon 1211). For total flooding and explosion suppression applications Halon 1301 is used and for local applications Halon 1211. These are based on methane where some of the hydrogen atoms are replaced with fluorine (F), bromine (Br), iodine (I) or chlorine (Cl). Halons are very efficient with only a 7 vol% concentration required for inerting a confined heptane fire. Halons are stored as condensed gases and therefore do not require a large storage volume. Halon 1301 is not especially toxic at extinguishing concentrations and can be used in rooms where people are present, however, exposure should be less than a couple of minutes. However, halons must be replaced for environmental reasons as they take active part in the depletion of the ozone layer. As a result of the Montreal Protocol, production of halons were phased out by the end of 1993 in the developed countries and they should be replaced before the end of 1997 in Sweden, except in some installations which have received exemption.

In Sweden the design of halon systems is regulated by the insurance companies code [RUS 170] until the end of 1997, after this date all halon systems should be replaced and no regulations are required. RUS 170 complies to a great extent with [NFPA 12A]. For explosion suppression systems no code has been available, in these cases the design is carried out according to the manufacturers' instructions. The design of a gaseous total flooding extinguishing system is based on the flame extinction, or inerting concentration. If the protected volume contains significant amounts of volatile liquid then the inerting concentration should be used. Due to the pressure increase as the agent is rapidly released, some compensation is needed as some is lost through openings, etc., in the room, the amount released is therefore increased by a factor of  $100/(100-C)$ . The design of the system must also compensate for the amount of agent disappearing through the ventilation system.

### Halon-like agents

Due to the phasing out of halons several halon-like agents have entered the market. In Sweden currently no design rules exist for these although internationally ISO14520 regulates 14. Halon-like agents have a low ODP factor, i.e. they do not take active part in the depletion of the ozone layer, they do however contribute to the global warming, i.e. they have a GWP factor in excess of 1. These agents are also more toxic than Halon 1301.

#### Carbon dioxide, CO<sub>2</sub>

Carbon dioxide is used for local and total flooding application. It is stored as a pressure condensed gas. The inerting concentration for CO<sub>2</sub> is 30-35 vol%, however, CO<sub>2</sub> is extremely toxic, humans become unconscious at a 10% vol. concentration and then die. One cannot therefore release CO<sub>2</sub> while people are present. In Sweden CO<sub>2</sub> extinguishing systems are designed according to [RUS 115]. In Europe CEN and CEA are developing new codes for CO<sub>2</sub>.

#### Inert gases

Nitrogen, argon, Argonite and Inergen are stored as compressed gases and therefore require a rather large storage volume. They are only used for total flooding applications. There are currently no design rules available for these gases in Sweden, but there will be before the end of 1997. CEA is currently working on a code for Inergen and Argon. The inerting concentration for nitrogen and argon is about 45%, at such high agent levels the oxygen concentration decreases which can be dangerous for people with a weak heart. Inergen is a mixture of 52% N<sub>2</sub>, 40% Ar and 8% CO<sub>2</sub>, the toxicity depends on the low oxygen concentration and the CO<sub>2</sub> content. Argonite is a mixture of 50% N<sub>2</sub> and 50% Ar, the toxicity of which depends on the low oxygen concentration.

### 4.1.2 Liquid agents

Water sprinkler are one of the most commonly used extinguishants, they are very useful for limiting the fire, but do not usually extinguish the fire completely. In some cases detergents are added to the water to produce a foam. Water is very cheap and has no toxic effect, but it causes water damage. Water sprinkler systems are designed so that a certain water density (l/min/m<sup>2</sup>) reaches the floor. If the building is high the sprinklers

are placed on several levels. In high rack storage buildings the sprinkler design is especially important. Design rules for this is available, in Sweden [RUS 120] and in USA [NFPA 13], while CEN is working on a European standard.

Water mist systems have recently become more popular. For such systems no design rules are presently available. Instead water mist systems are tested against specific fire scenarios. IMO was first to develop a test for ship cabins and restaurants (light hazard), and one for engine rooms. For the light hazard, control of the fire is required for approval, while in the engine room extinction is required. The Underwriters Laboratory has more recently developed a standard [UL 2167] similar to the IMO tests for "light hazards" (cabins, corridors) and also for "ordinary hazards" (tax-free shops). Factory Mutual has developed a test for gas turbines. At ISO work is being carried out to develop a standard based on the IMO and UL standard.

#### 4.1.3 Solid phase agents

Solid phase extinguishants are dry powders. Dry powders are extremely efficient as an extinguishing media against all types of fires, but require a lot of cleaning after use. They can almost only be used in dirty environments, and are very efficient in preventing dust explosions. Dry powders are very common in manual extinguishers and to some extent for local applications.

Dry powder total flooding systems are designed so that the design concentration is reached within the entire protected volume in less than 30s [NFPA 17]. Additional dry powder is required to compensate for losses due to openings and the ventilation in a room. For local application the codes are not very prescriptive.

## 4.2 Experimental measurement of inerting and extinguishing concentrations

When discussing extinguishing agents two different concentration levels are important, one is the inerting concentration, the other the extinction concentration. The inerting concentration is the concentration required to

prevent the growth of a combustion wave in any premixed fuel/air mixture. The extinction concentration is the concentration required to extinguish a diffusion flame, this concentration is always lower than the inerting concentration.

#### 4.2.1 Measurement of the inerting concentration

The inerting concentration is measured using explosion bombs. The extinguishing agent, the fuel and air is premixed in a bomb, i.e. a container capable of withstanding pressures, and then the mixture is ignited by a spark and the pressure developed measured using a rapid pressure transducer. The inerting concentration is then determined as the lowest concentration of agent producing a pressure increase lower than a predefined value. However, as pointed out in Paper IV this inerting concentration is dependent on the size of the container and the ignition energy of the spark, i.e. an energy rich spark in a small container will produce too high a value of the inerting concentration. A more precise standard for inerting concentration measurements is therefore required.

#### 4.2.2 Measurement of the extinction concentration

The extinction concentration has traditionally been measured using the burner cup method. Burner cups are cheap and require a small amount of extinguishing agent, however, the results from different burner cups differ. Another disadvantage is that it is difficult to transpose the results from this small scale method into the design for full-scale systems. In a burner cup the burner is placed within a tube and around the burner flows the air and extinguishing agent. The results obtained are dependent on the rate of fuel flow. For liquid and solid fuels the results also depend on the geometry of both the burner and tube.

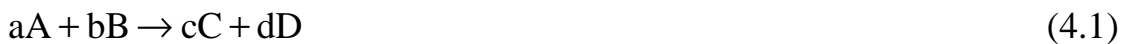
To overcome the scale problems with the burner cup method the tubular tube test was introduced. The tubular tube test consists of a tube burner where the agent and fuel is premixed before the outlet of the burner. The effectiveness of the agent is defined in terms of the REMP-value, the

Required Extinguishing Media Portion, i.e. the mass of extinguishing media required per unit mass of fuel.

### 4.3 Extinction theory

There is currently no model available which can predict whether a fire subject to a certain extinguishment system will be extinguished or not. The mechanism of extinction is complex and not yet fully understood. There are a few different processes that have to be considered when studying the extinction of fires. Extinction usually occurs due to removal of heat, but the removal of fuel or oxygen can also cause extinction, as well as chemical inhibition.

The rate of combustion of A for the reaction



is given by

$$-\frac{dA}{dt} = [A]^a [B]^b k \quad (4.2)$$

where  $[\ ]$  denotes concentration and the rate constant,  $k$ , is given by the Arrhenius expression

$$k = Ae^{-E_a/RT} \quad (4.3)$$

where  $E_a$  is the activation energy,  $R$  is the gas constant,  $T$  the temperature and  $A$  the frequency factor.

The combustion process can be reduced or stopped by removing heat, fuel or oxidiser, or by decreasing the rate constant. A diffusion flame can be considered as consisting of several very small premixed flamelets and therefore the theory above can be used for any flame. The combustion takes place in several steps, e.g. even for methane the combustion reaction is complex and can be divided into more than 50 steps. The rate constant can be considered as the overall rate constant of all the reaction steps at a particular temperature. If the reaction chain is interrupted then the rate constant decrease since the equivalent activation energy of the overall

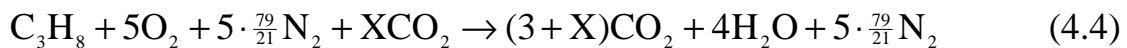
reaction rate has increased. The reaction chain can be interrupted by removal of one of the reactants in the chain, or by adding radicals which react with the reactants in the chain, so that other products are formed.

### 4.3.1 Thermal extinction theory

Most extinguishants act as inert gases, i.e. the heat produced from the combustion process is absorbed by the extinguishant. This mechanism is consistent with the observation that there is no decrease in the fire heat release rate as long as the amount of extinguishment agent added, is below a certain limit, and as soon as more extinguishment agent is added the fire is then extinguished.

As observed in equation 4.1 the combustion rate is very sensitive to the temperature. The inerting concentration can be calculated from the stoichiometric reaction formula of any fuel assuming a limiting adiabatic flame temperature of 1500-1600 K, i.e. below this temperature the reaction rate is so slow that it cannot sustain the combustion process.

For propane and carbon dioxide in air the reaction equation is;



If it is assumed that the limiting adiabatic temperature is 1550 K then the inerting concentration for CO<sub>2</sub> is 34 vol%.

### 4.3.2 Chemical inhibition

Halons and dry powders have some chemical inhibition effect, i.e. the rate constant is lowered by increasing the activation energy  $E_a$ . In halons the Br and I species scavenge the flame radicals and thereby interrupt the chemical reaction chain. Dry powders have a similar effect. This chemical inhibition effect means that the inerting concentration is lower than the concentration required from the thermal extinction theory. In addition, the rate of heat release from the flame is decreased at extinguishing agent concentrations below the extinction concentration.

### 4.3.3 Surface cooling

One important extinguishing mechanism when using water is the surface cooling. i.e. the water wets and cools the surface of the fuel so that no additional fuel evaporates to sustain the flame. This mechanism is valid for solid and liquid fuels. However, many liquid fuels are lighter than water and for these, the effect is minimal. For polar liquid fuels such as ethanol, water only dilutes the fuel and a lot of water is then required to decrease the rate of evaporation of the fuel.

### 4.3.4 Blowing

When the extinguishing agent is released into the room considerable turbulence is created. This could result in the flame being extinguished in the same way as a candle is blown out, i.e. the flame and the fuel are separated from each other. The turbulence also extends the combustion waves within the flame, which then lose more heat, if this becomes large enough the flame is extinguished [Lewis and vonElbe, 1961]. The turbulence in the room also causes the combustion gases to be recirculated into the flame, they can therefore extinguish the flame by acting as an inert gas.

### 4.3.5 A suppression model

A unified fire suppression model based on the "fire point" equation has been developed by [Beyler, 1992]. In this model the above mentioned extinction mechanisms can be included. In the equation the energy balance at the fuel surface is given by

$$\dot{m}'' = \frac{f\Delta H_c \dot{m}'' + \dot{Q}_E'' - \dot{Q}_L''}{L_v} \quad (4.5)$$

where  $\dot{m}''$  is the burning rate per unit area,  $f$  is the fraction of heat released which is transferred back to the fuel surface,  $\dot{Q}_E''$  is the external radiation,  $\dot{Q}_L''$  are the losses from the fuel surface. At the extinction limit  $f$  equals the fraction of heat that can be removed without extinguishing the flame. In

the absence of extinguishing agents this fraction varies between 0.1 and 0.4 depending on the reactivity of the fuel, it can be calculated using the limiting adiabatic temperature. The value of  $f$  decreases when using extinguishing agents that interacts with the flame, i.e. chemical inhibition, inerting and diluent effects are included in this term. The term  $\dot{Q}_L''$  includes the effect of surface cooling. Blowing affects the fraction  $f$ ; since if the flame and fuel is separated from one another, less heat is transferred from the flame to the fuel.

#### 4.4 Halon replacement

As previously mentioned the development of building codes is moving towards performance based fire codes. In addition, the phase out of Halon 1301 and 1211 now often requires performance based design to assure the previous protection level is still maintained. The evaluation process is shown schematically in figure 4.1. As can be seen several factors are included such as: the type of scenarios the agent should protect against, how soon the fire must be extinguished, if there are any people in the room, the importance of using a non-corrosive agent, if the agent should be electrically non-conductive and etc. Before the phase out of halons many of these factors were not taken into account since halons are so effective and have few disadvantages such as toxicity.

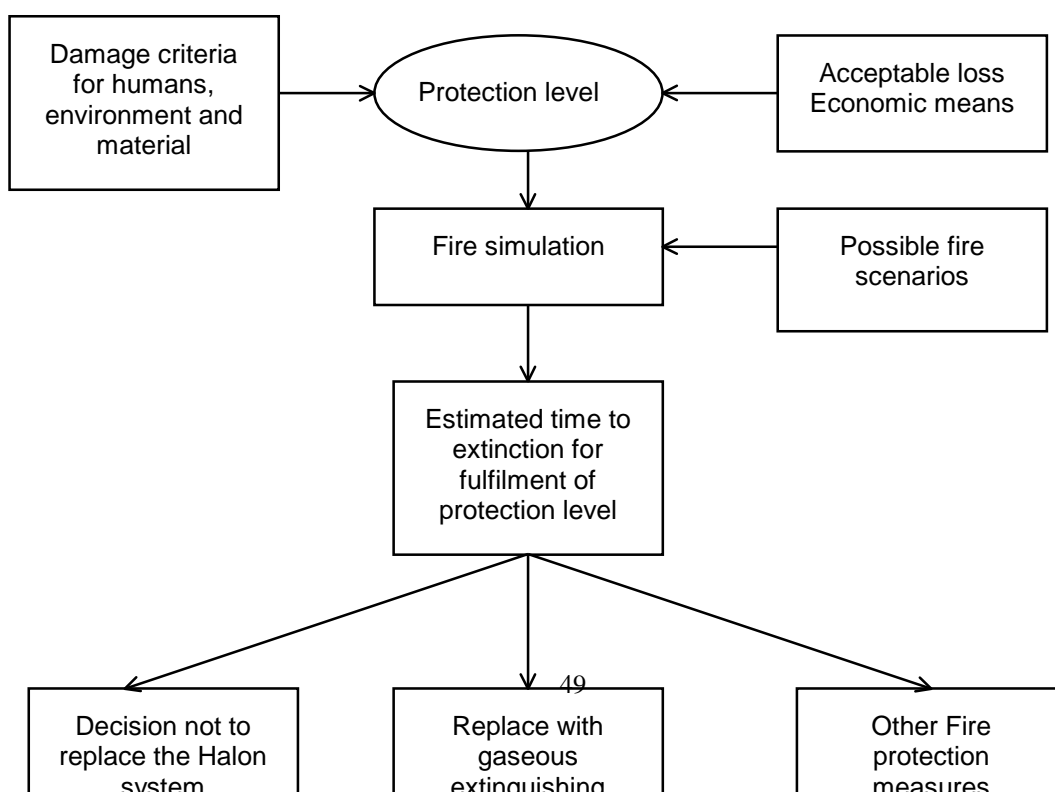


Figure 4.1. Halon replacement evaluation scheme.

Experience of halon replacement shows that one third of the systems are not being replaced, one third are replaced with some other gaseous extinguishing agent, and another third are replaced with better detection, sprinklers/water mist, dry powder or additional fire protection measures in the building design. When replacing with another gaseous agent there are two possible approaches, replace it with an agent that is similar to halon or replace it with another type.

In order to be certain that the protection level is attained it is desirable to be able to calculate whether a certain fire will be extinguished or not. However, no such models exist today. Instead, the extinction must be assured by correct design based on experience and fire tests. For extinguishing systems used over a long period such as water sprinklers, inert gases and dry powders the experience is often sufficient. However for "new" agents and systems such as water mist systems and the halon-like agents, little is known.

#### 4.4.1 Agents similar to halons

Considerable effort has been made to find agents similar to Halon 1301 and 1211. Several halocarbon compounds containing carbon, hydrogen, bromine, chlorine fluorine and iodine have been investigated. They are grouped into five types as follows: hydrobromofluorocarbons (HBFC), hydrofluorocarbons (HFC), hydrochlorofluorocarbons (HCFC), perfluorocarbons (FC or PFC) and fluoroidocarbons (FIC). They are all electrically non-conductive, can be stored as liquefied gases and are clean.

They are less efficient, produce more decomposition products and are more expensive than Halon 1301 [DiNenno, 1995].

All halon replacements produce more thermal decomposition products such as HF, than do Halons 1301 and 1211. In Paper IV the quantity of HF formed was shown to be proportional to the amount of fuel burnt while the extinguishing agent is present in the room. This shows that it is very important to release the extinguishing media into the room and extinguish the fire very quickly in order to decrease the amount of thermal decomposition products formed.

Another difficulty when it comes to halon replacements is that some of them are to some extent flammable when mixed with a fuel, i.e. when a small amount of extinguishing media is added to a flame, in a tubular burner test, the rate of heat release was found to increase, see Paper IV. This puts great demands on the design of the extinguishing system as it must ensure that enough extinguishing media reaches the fire in order to extinguish the flame and not increase the fire.

#### 4.4.2 Water mist

Liquid water is very efficient as an extinguishing media per unit weight. Experimental studies and thermal extinction theory suggest that liquid water is about twice as efficient per unit weight as Halon 1301. For the water to be as efficient as this, it is necessary for the water to evaporate completely while it is present in the flame; a water mist of small droplets is necessary. There are, however, several problems with distributing and maintaining the water mist in the whole protected volume as discussed in Paper V.

The inerting concentration for liquid water mist is  $280 \text{ g/m}^3$  protected volume and the extinction concentration for diffusion flames is  $140\text{-}190 \text{ g/m}^3$ . If the water is in the vapour phase twice this amount is required.

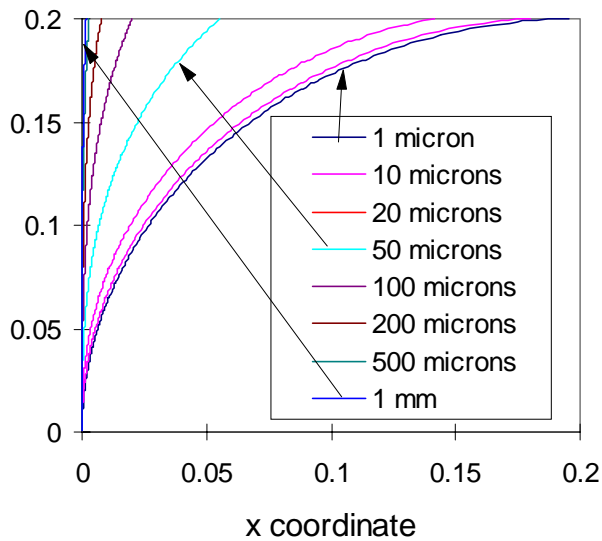


Figure 4.2 Trajectories for droplets of different sizes in an airflow of 4 m/s.

A high droplet momentum is required to reach the entire protected volume. This usually requires large droplets, but large droplets cannot reach obstructed areas. However, a high momentum can be obtained using small droplets of a high velocity. Water mists are usually produced by forcing water through a small nozzle producing a spray, the range of which is limited. The spray is soon retarded due to drag as the droplets can be considered as moving through the air. In order for the droplets to follow the general airstream pattern in a room and not hit obstacles like walls and machines, the droplets must have a diameter less than 20  $\mu\text{m}$ . The various trajectories of droplets of different size in an airstream directed towards a wall are presented in figure 4.2 above. Small droplets are difficult to produce, presently there is no water mist system commercially available which can produce droplets smaller than 20  $\mu\text{m}$ . This means that in order to cover the entire protected volume several nozzles are necessary.

Droplets tend to coagulate into larger droplets. The rate of coagulation is not especially high for droplets of equal size in still air. However, if the droplets differ in size, then the larger droplets will fall more rapidly due to gravity and drag and thus consume the smaller droplets. The change in droplet diameter as a function of time for a single droplet of initially 2 m in size in a mist consisting of 1 m droplets is shown in figure 4.3. As seen the droplet diameter increases rapidly once it has reached a critical limit. If there is turbulence the rate of coagulation will also increase.

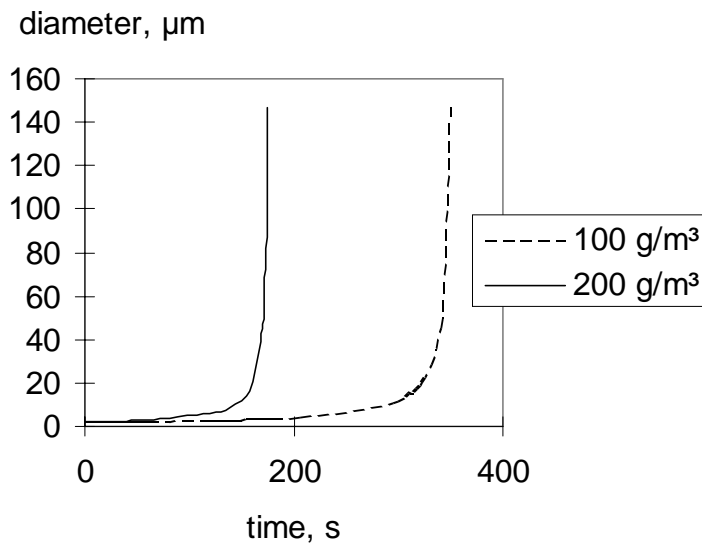


Figure 4.3 Droplet diameter as a function of time for a single droplet in a mist consisting of 1m droplets and a water content of 200 g/m<sup>3</sup> (solid line) and 100 g/m<sup>3</sup> (dotted line).

Small droplets have a very short lifetime. All small droplets will therefore quickly evaporate even at room temperature until the relative humidity is 100%. For extinction this means that an excess amount of mist must be produced over that predicted from the inerting and extinction limits.

Since water in vapour phase is lighter than air and liquid water is denser than air, the density of a water mist - air mixture is either heavier or lighter than air. Since no room can be completely sealed, air always comes into the room and the water mist will either lift or fall depending on its density. The amount of water in vapour phase is very temperature dependent. The density difference is therefore temperature dependent, which makes it difficult to design a water mist system capable of maintaining the water mist in suspension in the room for a few minutes. The density difference between dry and saturated air is illustrated in figure 4.4.

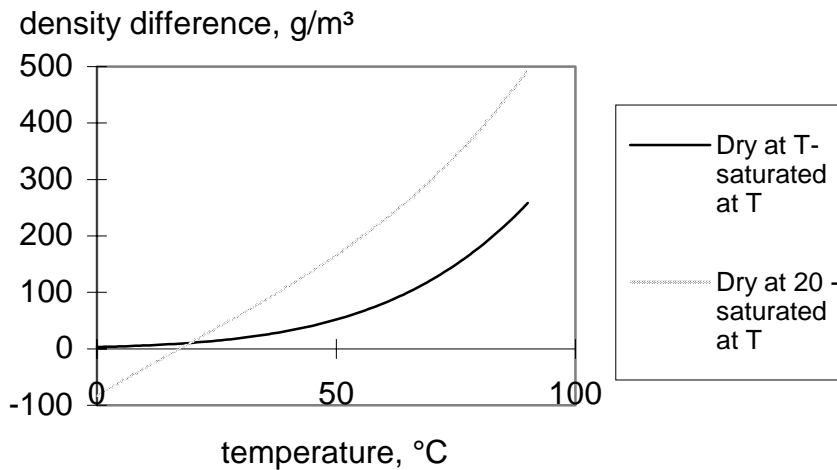


Figure 4.4 Density difference between dry air at T°C and saturated air at T°C (solid line) and density difference between dry air 20°C and water saturated air at T°C (grey line).

There is a very narrow window in which it is possible to use water mist as halon replacement. Small droplets are required (< 20µm) and also several nozzles in order to reach the entire protected volume. It is probably impossible to maintain the water mist concentration at a sufficiently high level during an adequate period to prevent reignition, without adding water continuously or in bursts. This will unfortunately increase water damage and water mists cannot be considered as clean agents.

As previously mentioned there are presently no design rules available for water mist systems. It is difficult to develop design rules since the extinction result of a water mist system is very scenario dependent; it depends on the location of the water mist nozzles, the fire and also whether there are any obstacles between the fire and the nozzles. To develop design rules it is essential to be able to determine the water content in the air. This can be accomplished using the instrument described in Paper VI. This measures the amount of water in both the vapour phase and also as small liquid droplets, it is not however suitable for use in the direct line of the spray. It has a short time constant, in the order of seconds, and has been found to be very stable and accurate over a period of several months without further calibration.

Basically two types of water mist systems are commercially available today, high-pressure systems and twin-fluid systems. High-pressure

systems force the water through a small nozzle, while twin-fluid systems mix the water with nitrogen. A third approach using super heated water was thought to convert the water mist system into a pressure condensed gas. The idea of a super heated water system is that, when the water at 130-170°C is released into the ambient environment, some of the water evaporates while the rest cools down, forming liquid droplets. However, no such systems have been found to function satisfactorily yet. There are problems with the amount of steam; too much is produced which would burn people present in the room. The large quantity of steam and the limited amount of small droplets are produced because the vapour pressure above a convex surface being much higher than the vapour pressure above a plane surface [Daniels and Alberty, 1961]. Small droplets are therefore very rapidly evaporated while the larger droplets grow. In order for a small droplet to be formed a condensation nuclei is needed, if no such nuclei are present the water will remain supersaturated.

Full scale experiments using different types of water mist systems are presented in Paper V which shows that the water content in the air is far too low for them to act as total flooding systems. Fires that are controlled, were found to be extinguished due to being hit directly by the nozzle spray, by flooding of the fuel container or simply wetting of the surfaces [Andersson and Holmstedt, 1996]. A typical example of the outcome of these tests is presented in figure 4.5. The water content in these experiments was measured using the instrument described in Paper VI.

Predicting whether a fire subject to a water spray or mist will be extinguished or not is a difficult task. It depends on the droplet size, velocity and the fire scenario. Some attempts have been made to model water droplets moving in the vicinity of a fire [Jackman, Nolan, Gardiner and Morgan, 1992]. This modelling however requires extensive information about the spray and droplets and extensive computer calculations.

Figure 4.5 Typical example of outcome of a full-scale test.

## 4.5 Concluding remarks

The process of extinction is not yet fully understood. Currently no model exists which can predict whether an extinguishing system can extinguish a certain fire.

In order to maintain the protection level of previous halon systems performance based designs are required. No replacement agent exists that has all the advantages of halons. The use of halon-like replacements, requires careful design, including a fast reliable detection and activation of the system, since they produce more thermal decomposition products than halons and can even increase the fire if not added fast enough. A rapid dispersion of the agent within the whole protected volume is also essential.

Some test methods for determining the extinction and inerting limits are especially dependent on the design of the equipment used. In addition, many of the tests are difficult to scale up, care must therefore be taken when using the results from tests in the design of practical systems.

Using water mists as halon replacements is difficult. No commercially available water mist system can be considered as a general total flooding system. All available systems can only be used for local application. However, a narrow window exists for water mist systems to be used as a

total flooding agent, the droplets must be small and of almost equal size. In addition the distribution of mist within the whole protected volume is essential, which almost certainly requires the use of several nozzles. No design rules presently exist for water mist systems. In order to be able to develop design rules for water mist systems it is essential to be able to measure the water content in air, an instrument suitable for this is described in Paper VI. Modelling extinction using water mist is complex and much remains to be carried out in this field.

## **5 Effect of Fires and Accidental Releases on Humans, the Environment and Components**

Humans, the environment and components can be affected by a fire or an accidental release by:

- pressure
- smoke and toxic or corrosive gases
- heat.

During the development and use of FREIA these have been found to be very weak links in the fire safety evaluation process using FREIA. In many of these areas very little is known.

### **5.1 Humans and the environment - Pressure**

Human beings are capable of withstanding relatively high dynamic pressures, if the pressure is static the human body is capable of withstanding even considerably higher pressures. When people are killed due to blast waves it is usually because objects fall on them. The pressure effects due to blast waves on humans are presented in Table 5.1 below [Fischer et al., 1995]. Pressure effects are also dependent on the impulse of the blast wave. In fires, pressures as high as those listed in Table 5.1 are seldom reached, except for smoke gas explosions. When it comes to accidental releases, a maximum pressure of 8 bar is produced if a premixed gas-air mixture is ignited inside a building, while on the outside pressures of the same order of magnitude are produced if the release results in an UVCE. Even higher pressures are produced if the release results in a detonation both inside and outside of buildings. Detonations are, however, very rare. Usually it is difficult to predict the pressures produced. In addition, the consequences for humans are very dependent on whether there is something nearby that can hit them. It is not therefore worth the effort involved to find better values for pressure effects on humans.

Pressure effects are usually limited to a small area and the effect of pressure on the environment is therefore seldom discussed. However, the same discussion as for humans is also valid, for both the general environment and animals; namely any adverse effect or injury are more dependent on being hit by a flying object.

Table 5.1 Pressure effects on humans

Pressure	Effect
35 kPa	Limit for eardrum rupture
70 kPa	Limit for lung damage
100 kPa	50% eardrum rupture
180 kPa	1 % mortality
210 kPa	10% mortality
260 kPa	50% mortality
300 kPa	90% mortality
350 kPa	99% mortality

## 5.2 Components - Pressure

Data on the effect of pressure on components such as machines are very rare and usually they can be considered as unaffected by pressure if they are solid. However, if they contain cavities they are more sensitive to pressure variations. When it comes to building sections such as windows, walls and doors, acceptable data does exist, Table 5.2 lists typical failure pressures of such elements [Harris, 1983].

Table 5.2 Typical failure pressures of some building elements

Element	Typical failure pressure (kPa)
Glass windows	2-7
Room doors	2-3
Light partition walls	2-5
50 mm thick breeze block walls	4-5
Unrestrained brick walls	7-15

## 5.3 Humans and the environment - Toxic effects

Toxic effects is a complex field. There is generally little data on the toxic danger for humans since it would be unethical to undertake such experiments. Instead one has to extrapolate from values obtained from experiments on animals, the results are however very uncertain. It is, however, possible to find published values on when eyes start to flood with tears, as well as other relevant information.

For some chemicals data is available to estimate percentage of deaths using the so called probit function

$$Pr = a + b \cdot \ln(C^n t) \quad (5.1)$$

where a, b, and n are chemical specific constants, C is the concentration in ppm and t is the exposure time in minutes. Pr is the probit variable which is a normal distribution and has a mean value of 5 and a standard deviation of 1. The probit value can be obtained from the cumulative normal distribution using the expression

$$Pr = \text{standard deviation} + 5.0 \quad (5.2)$$

The values for a, b and n are presented in Table 5.3 which can be used in the above function. These values are estimated from animal experiments. When no values are available one can only roughly estimate the value of the dangerous dose or concentration.

Table 5.3 Constants for the Lethal Probit Equation

Substance	a	b	n
Acrolein	-9.931	2.049	1
Acrylonitrile	-29.42	3.008	1.43
Ammonia	-35.9	1.85	2
Benzene	-109.78	5.3	2
Bromine	-9.04	0.92	2
Carbon monoxide	-37.98	3.7	1
Carbon tetrachloride	-6.29	0.408	2.5
Chlorine	-8.29	0.92	2
Formaldehyde	-12.24	1.3	2

Substance	a	b	n
Hydrogen chloride	-16.85	2.0	1.0
Hydrogen cyanide	-29.42	3.008	1.43
Hydrogen sulphide	-31.42	3.008	1.43

Table 5.3 Continued

Substance	a	b	n
Methyl bromide	-56.81	5.27	1.0
Methyl isocyanate	-5.642	1.637	0.653
Nitrogen dioxide	-13.79	1.4	2
Phosgene	-19.27	3.686	1
Propylene oxide	-7.415	0.509	2
Sulphur dioxide	-15.67	2.1	1.0
Toluene	-6.794	0.408	2.50

Several different toxic limits are available in the literature. One of the most common is IDLH (Immediately Dangerous to Life or Health). Swedish authorities use the term "Hygienic Threshold Limit" for regulating the environment for the workers in industry. Similar regulations are available in other countries. The Hygienic Threshold Limit is a time weighted mean value of the substance in the air. The limits are presented as a concentration that a human can be subject to for the whole working day, for a lifetime, without noticeable effects and also a short time exposure limit which is safe for time-periods of less than 15 minutes. The Hygienic Threshold limits are estimated from experience in working life, experiments using volunteers, animal tests and also by comparison with substances of similar chemical properties. These values are based on the knowledge about the chemical to date, which of course can change. For instance, vinyl chloride was considered a relatively harmless substance and the hygienic threshold limit was set to 500 ppm. More recently it was found that vinyl chloride causes a certain form of liver cancer and the limit was lowered to 3 ppm. The IDLH level represents the maximum airborne concentration of a substance, to which a healthy male worker can be exposed for as long as 30 minutes and still be able to escape without loss of life or irreversible organ damage.

Several of the toxic limits are estimated from animal experiments which result in values such as LC<sub>50</sub>, LD<sub>50</sub>, LC<sub>10</sub>, LD<sub>10</sub>. The LC<sub>50</sub> and LC<sub>10</sub> values concentrations which results in 50% and 10% deaths respectively. The experiments are performed in such a way that the animals are divided into several groups, each group is subject to a certain airborne concentration of the substance for a specified time. After the specified time the LC<sub>50</sub> value is determined as the concentration which caused 50% deaths within a group. The LC-values will vary depending on the duration and the species involved in the experiments. The certainty of the value is very dependent on the number of animals in the test. The LD-values represents the lethal dose. In these experiments the substance is either injected in a vein, in the stomach or added to the food. The outcome of the experiments will vary depending on whether the substance was injected or consumed as the food. What species used will also influence the LD-value. Of course there are large uncertainties involved when extrapolating the LC<sub>50</sub>, LD<sub>10</sub>, etc. values into IDLH, etc. for humans. Most experiments are conducted using rats and mice, but in some cases rabbits, dogs, pigs and monkeys are used.

Estimating the consequences for humans due to exposure to several gases at the same time is a difficult task. NIST [Babrauskas et al., 1991] has invented a model for calculating LC<sub>50</sub> values due to exposure of several gases at the same time, which have more recently been extended by Risö [Smith-Hansen, 1994]. In this model the effect of oxygen depletion, CO, CO<sub>2</sub>, HCN, HCl, HBr, NO<sub>2</sub>, SO<sub>2</sub>, Acrolein, Formaldehyde, NH<sub>3</sub>, NO, COCl<sub>2</sub>, CS<sub>2</sub>, COS and H<sub>2</sub>S are included. All toxic effects are assumed to be additive and no account is taken of synergetic effects. The model is used to estimate an acute LC<sub>50</sub> value for a substance subject to combustion, the LC<sub>50</sub> (g/m<sup>3</sup>) value is given by

$$LC_{50} = \frac{\Delta m}{FED \cdot V} \quad (5.3)$$

where m is mass loss per time unit in g, V is total air volume per time unit and FED, the Fractional effective Exposure Dose is given by

$$FED = \frac{d[CO]}{[CO_2] - b} + \frac{[HCN]}{LC_{50}(HCN)} + \frac{21 - [O_2]}{21 - LC_{50}(O_2)} + \frac{[HCl]}{LC_{50}(HCl)} + \frac{[HBr]}{LC_{50}(HBr)} + \frac{[NO_2]}{LC_{50}(NO_2)} + \frac{[SO_2]}{LC_{50}(SO_2)} + \dots \quad (5.4)$$

where [ ] denotes measured concentration. The first term expresses the increased potency of CO due to CO<sub>2</sub>, d and b depends on the CO<sub>2</sub> concentration.

For the estimation of environmental effects the situation is even worse. Some species can be extremely sensitive to a certain chemical. Animals can be exposed to the chemicals in different ways compared to humans. Even an earthworm can be very important in an ecological system, if all earthworms are killed then several plants could be extinct, since the decomposition rate of dead plant material would decrease, which in turn leads to a reduction in the rate of nutrient release into the soil.

Ecologists and politicians have tried to estimate a safe concentration for several chemicals. This defines a limit on global species extinction of not more than 5% with a statistical certainty of 95%. However, this approach is subject to much discussion.

## 5.4 Components - Corrosive effects and smoke

Normal fires seldom produce sufficient corrosive products to affect components in a fire room. However, fires in chemical storage areas may result in formation of significant quantities of corrosive products. The thermal decomposition products from both halon and halon replacements are corrosive. Corrosive damage can also be caused by the accidental release of stored chemicals.

Smoke consists of aerosols and tar which can damage textiles and cause materials to smell. In addition, the soot in the smoke can induce electrical currents in electronic equipment. No attempts have been made to model these effects due to smoke.

## 5.5 Humans and the environment - Heat

In FREIA the effect of heat on humans is given as distances which produce first, second and third degree burns outside buildings, no calculations are performed within the building. The radiation levels for first, second and third degree burns are chosen according to [Räddningsverket, 1989].

To estimate the number of fatalities a probit function can be used [CPQRA, 1989; Whazan, 1988]. The number of fatalities will of course depend on what people in the vicinity are wearing and whether they can find shelter. The probit function does not take this into account.

The computer code ICARUS (Injuries Caused by Radiation Upon the Skin) evaluates the time to second degree burn injury due to thermal radiation [Bamford and Boydell, 1995]. It takes into consideration the shielding effects of clothing. This model requires input data on the thermal properties of the clothing, their thickness and the air gap between the layers. Second degree burns are assumed to occur when the damage integral reaches the value of 1. The damage integral is calculated from

$$\frac{d\Omega}{dt} = 1.43 \cdot 10^{72} \exp\left(\frac{-4.61 \cdot 10^5}{8.31T}\right) \quad (5.5)$$

where T is the temperature at the epidermis-dermis interface, i.e. the epidermis basal layer depth of 80µm. When this temperature is below 44°C no addition to the damage integral is made.

The ICARUS model requires considerable data on clothing characteristics which is seldom known. In Paper VII a human skin simulator, a test dummy, is described. This is made of plastic with the same thermal characteristics as human skin, as well as a blood circulation system. The damage criteria used is from [Bull and Lawrence, 1979]. They found that a skin temperature of 74°C for more than 1 second is a threshold limit for burns. If the temperature reaches 98°C in 1 second third degree burns occur. A skin temperature of 60°C for 10 seconds also results in burns. However, as discussed in Paper VII, comparing different burn criteria is complicated. Care must be taken of whether it is the skin surface temperature or another temperature such as the temperature at the epidermis-dermis interface that decides the damage criteria.

The test dummy has been very valuable when testing the effect of different fire scenarios on humans and also to determine how fast the extinction system must react to prevent injury. It has also been used in the extinction tests with the superheated water.

## 5.6 Components - Heat

As previously described FREIA uses a dose concept which assumes that all components have a certain impact level below which no damage occurs (see chapter 2.4). All dosages above this level are integrated and compared to the critical dose. However, this approach has not been fully tested except for some types of cables [Frank and Moieni, 1986]. Improving the model would require expensive experimental investigations, unfortunately no funding is available for this. The manner in which the various heat fluxes are added together in FREIA is not very rigid. However, data for use in FREIA is available from the ISO ignitability test for building materials and linings.



## **6 Conclusions and Suggestions for Future Work**

The computer package FREIA has been found to be a valuable tool for conducting fire hazard analysis of industrial premises using engineering techniques. It evaluates the consequences of fires and/or any accidental release on components and humans within and in the vicinity of the plant. Evaluating the effect on the environment is more difficult and FREIA has only limited facilities for undertaking this. FREIA is especially valuable when the plant contains a limited number of very important and vulnerable components. In this case it can be enough to move a component slightly, or put up a shield to protect a certain component, to considerably increase the compartments fire safety margin.

There are, however, some areas in the fire hazard evaluation chain in FREIA that require improvement. These are fire spread, fire detection, extinguishing and effect of fire and accidental release on humans, the environment and components. In addition, in order for FREIA to be considered an established risk analysis tool, statistical information on initial fires and fire development, as well as uncertainties in data ought to be included in the system more comprehensively.

### Fire spread

In FREIA the user has often to specify the rate of heat release curve. It would be more appropriate if this could be directly calculated. Fire spread is an area where considerable research is taking place and still more remains to be carried out. However, this has not been discussed in this thesis.

### Detector activation

FREIA includes the two-zone model, FIRE SIMULATOR. Such models cannot take into consideration complex room geometries, sloping ceilings, porous false ceilings, the local effects of ventilation, or beams in the ceiling. To do this, CFD models are required. CFD-models can predict heat detector activation reasonably well. However, for smoke detectors this is more difficult. There is currently no model available which predicts whether a smoke detector subject to a certain flow of smoke is activated or

not. In addition, the soot models for use in the CFD models are still under development. Possible approaches when modelling the smoke field is to assume that it closely correlates with the temperature, O<sub>2</sub>, CO<sub>2</sub> or the CO field; or to treat it as an inert gas, by assuming that a certain fraction of the fuel is converted to soot. Experiments show that the above concentration fields closely agrees with one another. Attempts to simulate tests according to the EN54 standard, assuming that the smoke and oxygen depletion are correlated, resulted in close agreement between test and simulation for some of the fires, however in others the results differed by a factor of three. This can, however, probably be explained by the wavelength dependence of light obscuration measurements. A simulation of the soot volume fraction in a propylene fire plume, where the soot was treated as an inert gas and where 10% of the fuel was assumed to be converted into soot, resulted in an estimated soot volume fraction which is close to a factor of three less than that found experimentally. There are, however, several problems with measuring the soot volume fraction, and the experimental uncertainty is close to a factor of three. Considerable research is still needed to solve the problem of predicting smoke detector activation. Models are especially needed for smoke detector response, and the soot models also require improvement.

### Extinguishment

There is currently no extinguishing agent available that can completely replace halons. Special care must therefore be taken of several factors when considering any replacements. These would include the level of fire protection, the need for a clean agent and the presence of people in the room. All halon-like replacement agents produce more toxic thermal decomposition products than Halon. The design of these systems is therefore very important. In addition, many of the agents are flammable when mixed with fuel at concentrations less than the extinction concentration.

Water mist has recently been mentioned as a possible halon replacement. There are however no systems presently available on the market which can fulfil the requirements of a total flooding system. A very narrow window exists in which water mist can act as a total flooding system. All droplets must be small (< 20  $\mu$ m) and of equal size. Water must be added continuously, or in bursts, in order to maintain a sufficient water content.

In addition more research is required in order to be able to model and predict whether an extinguishing system extinguishes the fire, only limits it or leaves it unaffected.

#### Effect of fires and accidental releases

Estimating the effect of fires and accidental releases on humans, the environment and components is a complex field. Pressure damage is, to a large extent, dependent on whether there is anything nearby that can hit the evaluated area. However, pressure damage is usually very local and therefore research in this area is not of such great importance. Toxic, corrosive and smoke damage is an area where much remains to be done. Little is known about the gases and smoke produced in fires, research has recently begun in this field. In addition, estimating toxic effects on humans and the environment is very complex. In the case of corrosive effects the situation is better. Little is known about aerosols, tar and soot produced in fires and their deposition on for instance textiles and electrical equipment, this is an area where much remains to be investigated. In FREIA a dose model for estimating damage on components is used, this has not been validated. Human skin burns are very dependent on the clothing being worn. Mathematical models for taking this into consideration are complex. A human skin simulator has therefore been developed, which is described in this thesis. The simulator has been found to be valuable in fire tests as well as extinguishing tests.



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Finally, I have chosen to dedicate this work to my horse Dimma. During these years she has relieved me from so much frustration. Whatever the hour she always greeted me with joy and after only a couple of minutes with her, my mind was clear and all the problems gone. I always promised her that when my thesis was finished we would spend lots of time together. But now that the thesis is finished, she is grazing in the eternal green grass.



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## Appendix A

### The Release of Hazardous Substances



## Nomenclature

AA	discharge area, m <sup>2</sup>
A <sub>f</sub>	flame area, m <sup>2</sup>
A <sub>o</sub>	opening areas, m <sup>2</sup>
A <sub>p</sub>	liquid pool area, m <sup>2</sup>
A <sub>s</sub>	area on which vent is placed, m <sup>2</sup>
A <sub>v</sub>	vent area, m <sup>2</sup>
B	mass transport number
C	parameter in evaporation model
C <sub>d</sub>	the discharge coefficient, $0.6 \leq C_d \leq 1$
C <sub>o</sub>	initial concentration, often 100%
C <sub>p,air</sub>	C <sub>p</sub> of air, J/kg/K
C <sub>pl</sub>	C <sub>p</sub> of liquid phase, J/kg/K
$\bar{C}_x$	average concentration at (x, r)
c <sub>gr</sub>	ground c <sub>p</sub> , typical value 1000 J/kg/K
D	diameter of pool or pipe, m
D <sub>B</sub>	diameter of BLEVE, m
d	fragment diameter, inches
d <sub>o</sub>	initial diameter of jet, discharge diameter, m
E <sub>av</sub>	average emissive power, kW/m <sup>2</sup>
E <sub>c</sub>	heat of combustion of gas
E <sub>c TNT</sub>	heat of combustion of TNT ( 4450 kJ/kg)
E <sub>m</sub>	the maximum emissive power of luminous spots ( 140 kW/m <sup>2</sup> )
E <sub>S</sub>	emissive power of smoke ( 20 kW/m <sup>2</sup> )
F	is a friction factor taken from Table 1
F <sub>h</sub>	horizontal view factor
F <sub>max</sub>	maximum view factor
F <sub>v</sub>	vertical view factor
Fr	Froude number
F <sub>v</sub>	flash fraction
g	9.81 m/s <sup>2</sup>
H	the liquid head (m) above releasing point
H	flame height, m
H <sub>B</sub>	height of BLEVE above ground, m
h	convective heat transfer coefficient, W/m <sup>2</sup> /K
I	radiation, kW/m <sup>2</sup>
K	vent coefficient
k <sub>air</sub>	conductivity of air (0.026 W/m/K)
L <sub>f</sub>	jet flame length, m

$L_p$	pipe length, m
$M$	molecular weight, kg/mole
$M_{air}$	molecular weight of air (0.0288 kg/mole)
$M_F$	molecular weight of fuel, kg/mole
$m$	mass of flammable gas, kg
$m$	released mass, kg
$\dot{m}$	discharge rate, kg/s
$\dot{m}'' C$	burning rate of pool, here assumed to be equal to $\dot{m}''_{\infty}$
$m_e$	total evaporated mass, kg
$\dot{m}_{ev} D$	mass loss from pool, kg/s
$N$	non-equilibrium correction factor
$n$	ratio of the number of moles of reactants to that of products for the stoichiometric mixture
$Nu$	Nusselt number
$nr$	number of fragments
$P_b$	rupture pressure, psig
$P_s$	the vapour pressure of the substance, atm
$P_{sh}$	vapour pressure of hydrazine, atm
$p$	the pressure of the container, Pa
$p_1$	first pressure peak, mbar
$p_2$	second pressure peak, mbar
$p_a$	the ambient pressure, Pa
$p_F$	vapour pressure of fuel
$p_f$	final pressure of expanded gas, psia
$p_i$	initial pressure of compressed gas, psia
$Pr$	Prandtl's number
$Q_a$	volumetric ventilation rate, m <sup>3</sup> /s
$Q_g$	volumetric flow of gas into room, m <sup>3</sup> /s
$q_e$	total emissive radiation, W
$q_{loss}$	cooling of gas, J/s
$R$	gas constant (8.3143 J/mole/K)
$R_R$	gas constant (1.987 Btu/lb mole/°R)
$r$	stoichiometric air/fuel ratio
$r$	distance, m
$Re$	Reynolds number
$r_i$	initial air/fuel ratio
$r_{max}$	the maximum radius of the pool, m
$s$	parameter in evaporation model
$S_e$	experimentally determined parameter ( 0.12 /m )
$T$	temperature, K

$T_1$	temperature of compressed gas, °R
$T_{amb}$	ambient temperature, K
$T_{bp}$	the normal boiling point of the substance, K
$T_F$	temperature correction factor
$T_f$	flame temperature, K
$T_g$	gas temperature, K
$T_{g\ av}$	average gas temperature, K
$T_{gi}$	initial gas temperature, K
$T_i$	initial temperature, K
$T_o$	standard temperature (492°R)
$T_p$	temperature in degrees Celsius
$T_s$	storage temperature, K
$t$	time, s
$t_B$	duration of BLEVE, s
$t_{eff}$	effective duration of flash fire, s
$u$	windspeed, m/s
$U_0$	initial velocity, ft/s
$U_o$	initial velocity of gas, m/s
$u^*$	non dimensional windspeed
$V$	room volume, m <sup>3</sup>
$v$	the discharge velocity ( $m/\rho_v/A$ ), m/s
$V_f$	Volume of flash fire, m <sup>3</sup>
$V_g$	volume of compressed gas, ft <sup>3</sup>
$V_{in}$	volumetric flow of gas into room, m <sup>3</sup> /s
$V_{out}$	volumetric flow of gas out of room, m <sup>3</sup> /s
$V_{vessel}$	the volume of the vessel, m <sup>3</sup>
$\dot{V} F$	the volumetric discharge rate into the pool, m <sup>3</sup> /s
$W$	energy in lb or kg TNT
$W$	weight per unit area of vent cladding, kg/m <sup>2</sup>
$W_f$	weight of fragments, lb
$x$	distance, m
$Y_{F4}$	mass fraction fuel in air above pool
$Y_{FR}$	mass fraction fuel in pool
$Y_{FW}$	mass fraction fuel in gas phase at liquid surface
$\cap$	parameter in flash fire model
$\exists$	turbulence factor
$($	gas specific heat ratio (Cp/Cv)
$H_c$	Heat of combustion, J/kg
$)H_v$	heat of vaporisation of release, J/kg
$)P$	over pressure, Pa

$\Delta T$	$(T_{\text{source}} - T_{\text{ambient}}), \text{ K}$
$\Delta T$	$T_s - T_{\text{bp}}, \text{ K}$
$\epsilon$	emmissivity of hot gas taken as 1.0
$\theta$	empirical explosion factor [ 0.01 - 0.1] here taken to be 0.1
$\alpha$	flame tilt
$\delta$	thermal conductivity of ground, typical value 1W/m/K
$\nu$	kinematic viscosity of air ( $15.08 * 10^{-6} \text{ m}^2/\text{s}$ )
$\Delta$	ground density, typical value $2*10^3 \text{ kg/m}^3$
$\Delta_a$	air density
$\Delta_g$	gas density
$\Delta_l$	liquid density, $\text{kg/m}^3$
$\Delta_p$	gas density in container, $\text{kg/m}^3$
$\Delta_v$	the density of air at the appropriate temperature
$\Phi$	the Stefan Boltzmann constant ( $5.76 * 10^{-8} \text{ W/m}^2\text{K}^4$ )
	transmissivity

## The Release of Hazardous Substances

This appendix describes the models used in the release scenario section of the program FREIA, it is divided into four sections. The first describes the calculational flow of the program and the basic principles of how to evaluate the consequences of an accidental release. The next describes models used in both indoors and outdoors scenarios, that is basically the source modelling. The third describes the models used in the outdoor scenarios and the final section those used indoors.

### 1 Calculational flow in FREIA

The package FREIA evaluates the consequences of released flammable and/or toxic gases, liquefied gases and liquids both indoors and also outdoors. The models included in the package are well established, with many of them based on empirical equations. All these do of course have their own particular restrictions. FREIA, however, tries to use these models in the most appropriate way and also estimates values when they are outside their validity range.

Evaluating the consequences of a discharged hazardous substance is a rather complicated process. A typical event tree for the release of a hazardous substance outdoors is shown in figure 1 with each box in this requiring modelling. For the indoor scenario a similar tree exists, however, this does not contain UVCE (Unconfined Vapor Cloud Explosion), flash fire and BLEVE (Boiling Liquid Expanding Vapor Explosion), but instead includes boxes for both inside and physical explosions.

Estimating the consequences is basically carried out in four steps. These include modelling:

- the source (instantaneous source, continuous discharge rate, formation of a liquid pool and evaporation),
- the dispersion (jet dispersion, cloud dispersion),
- the ignition (jet flame, flash fire, pool fire, explosion) and finally
- the impact (radiation, toxic, pressure).

As can be seen in figure 1 some scenarios exclude others, for instance if there is a pool fire then no cloud dispersion occurs. FREIA, however, evaluates all possible branches of the event tree during one execution, since

in most instances it is interesting to know all the consequences, whether or not there are any ignition sources present.

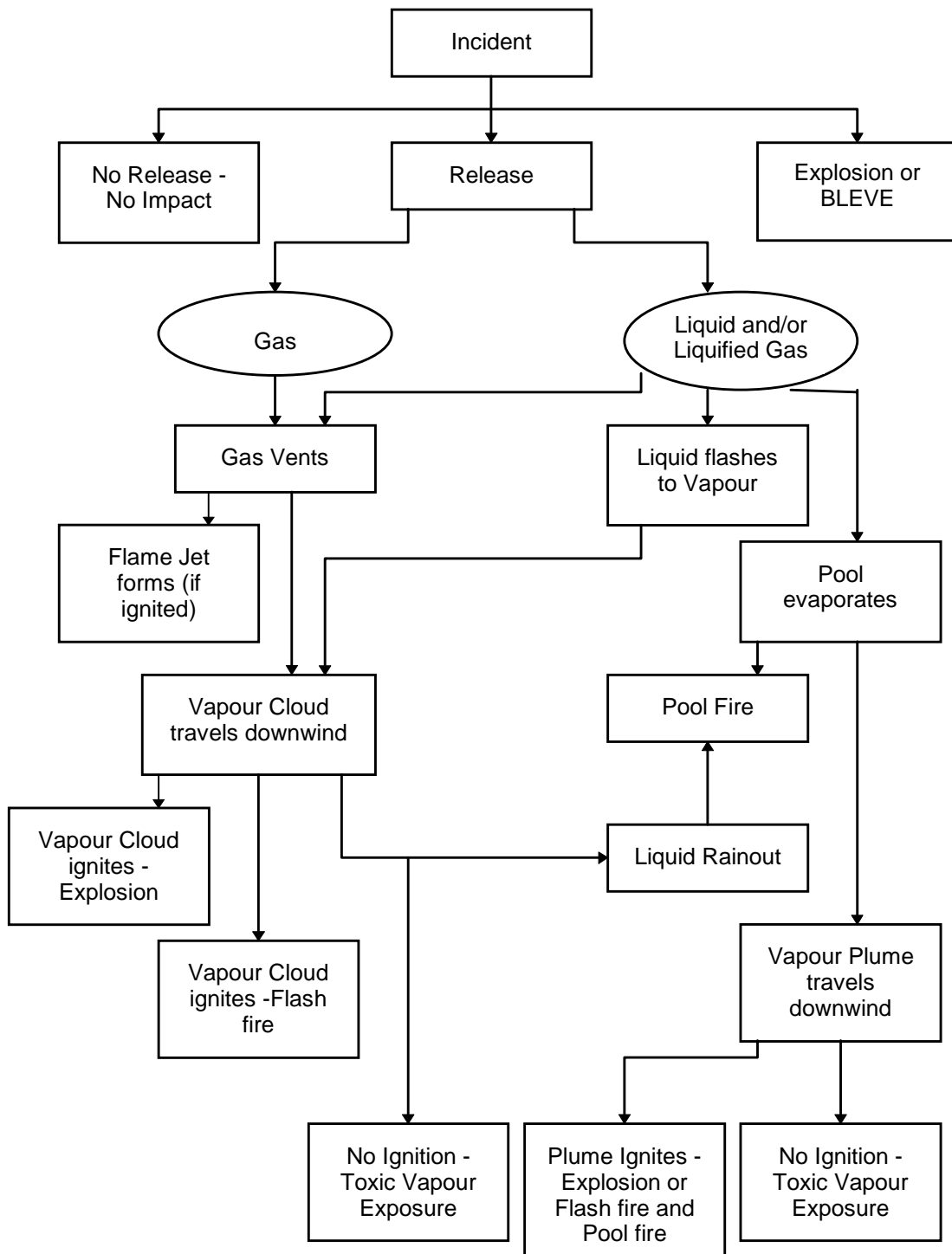


Figure 1. Event tree for release outdoors.

The calculational flow in FREIA is controlled by a shell built up of several rules. These rules select which of the models is to be used and to some extent the input data given to them. From the results of one model the rules decide which model to use next and the input data for that model.

## 2 Models used both indoors and outdoors: the source models

The quantity released can be specified as either instantaneous or continuous. For an instantaneous release one has only to specify the mass released. In the continuous case the source is specified as a discharge rate. The discharge rate is often unknown and must therefore be calculated by utilising the pressure, temperature and hole configuration of the discharge. If the discharge is in the liquid phase, then a liquid pool could form and then the evaporation rate of the pool must be calculated.

It is often difficult to distinguish between a continuous and an instantaneous release. It is the transport time for the discharge to reach the area where the actual consequences are being evaluated and also the discharge duration that decides whether the release is continuous or not. In most cases discharges lasting less than 10 seconds should be considered as instantaneous and those lasting more than 30 seconds considered continuous. At the end of each execution FREIA calculates the transport time and compares it with the duration of the discharge and produces a warning if the incorrect release scenario has been chosen.

### **Discharge rate**

When estimating the discharge rate one has to distinguish between the following three different situations, a gas, a liquid or a two-phase discharge, these are illustrated in figure 2. The single phase discharge rate calculations (gaseous and liquid), are carried out according to well established physical equations, while for the two-phase situation several different models exist.

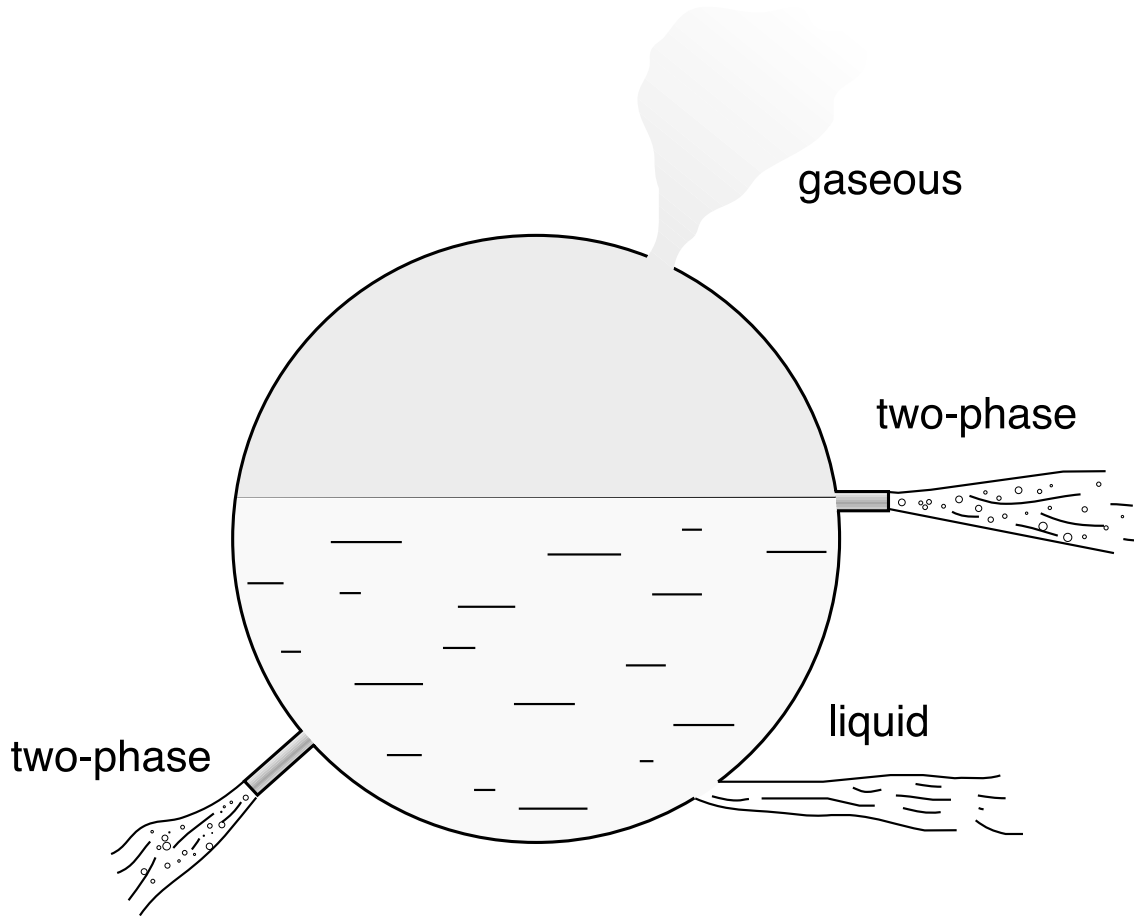


Figure 2. Schematic diagram of gaseous, liquid or two phase discharges.

### Gas discharge

The gas discharge is assumed to occur from a infinitely large pressure tank which thus produces a constant rate of discharge,  $\dot{m}$ . However, this is seldom true, but inspite of this, all subsequent models will use only a constant rate of discharge and by so doing the "worst case" scenario is evaluated. If it is of interest to calculate the correct discharge rate then the pressure term in the formulas below (1, 3) must be modified.

For sonic flows the discharge rate  $\dot{m}$  (kg/s) is given by [1]

$$\dot{m} = C_d \cdot A \cdot p \sqrt{\frac{\gamma M}{RT}} \cdot \left[ \frac{2}{\gamma + 1} \right]^{\frac{(\gamma + 1)}{\gamma - 1} \cdot \frac{1}{2}} G \quad (1)$$

where  $C_d$  = the discharge coefficient,  $0.6 \leq C_d \leq 1$

- A = the area of the hole, m<sup>2</sup>
- p = the pressure of the container, Pa
- ( = gas specific heat ratio (C<sub>p</sub>/C<sub>v</sub>)
- M = molecular weight, kg/mole
- R = gas constant ( 8.3143 J/mole/K)
- T = temperature in container, K

C<sub>d</sub> is dependent on the shape of the hole and is equal to 0.98 for a safety valve and 0.6 for a circular hole with sharp edges.

Sonic flow is established when

$$p / p_a \geq \left[ \frac{\gamma + 1}{2} \right]^{\gamma / (\gamma - 1)} H \quad (2)$$

where p<sub>a</sub> = the ambient pressure, Pa

For subsonic flows the discharge rate is given by

$$\dot{m} = C_d A \sqrt{2 \rho_p p \frac{\gamma}{\gamma - 1} \left( \frac{p_a}{p} \right)^{2/\gamma} - \left( \frac{p_a}{p} \right)^{\frac{\gamma + 1}{\gamma}} I} \quad (3)$$

where Δ<sub>p</sub> = the gas density in the container, kg/m<sup>3</sup>.

### Two-phase and liquid discharge rate

For two-phase and liquid discharges the model of Fauske and Epstein [2] is used. This takes into consideration the pipe length L<sub>p</sub> and diameter D through which the liquid flows from the container. This model is the most commonly used to calculate the two-phase discharge rate. When the length L<sub>p</sub> is equal to zero a liquid discharge occurs. The discharge rate ṁ for saturated liquids (that is pressurised gases) is given by (4), when L<sub>p</sub> > 0.1 m.

$$\dot{m} = F \frac{A \Delta H_v}{\frac{1}{\rho_p} - \frac{1}{\rho_l}} \frac{1}{\sqrt{T_s C_{pl}}} , L_p > 0.1 \text{ m J} \quad (4)$$

where  $F$  = is a friction factor taken from table 1  
 $A$  = is the discharge area,  $m^2$   
 $\Delta H_v$  = heat of vaporisation, J/kg  
 $\Delta \rho_p$  = gas density in container,  $kg/m^3$   
 $\Delta \rho_l$  = liquid density in tank,  $kg/m^3$   
 $T_s$  = storage temperature, K  
 $C_{pl}$  =  $C_p$  of liquid phase, J/kg/K

Table 1. The variation of the friction factor  $F$  as a function of the pipes length to diameter ratio ( $L_p/D$ )

Length to diameter ratio ( $L_p/D$ )	Friction factor ( $F$ )
0	1
50	0.85
100	0.75
200	0.65
400	0.55

When  $L_p < 0.1m$  no equilibrium two-phase flow will be established and the discharge rate  $\dot{m}$  is given by

$$\dot{m} = \frac{1}{\sqrt{N}} \frac{A \Delta H_v}{\frac{1}{\rho_p} - \frac{1}{\rho_l}} \frac{1}{\sqrt{T_s C_{pl}}} , L_p < 0.1m \quad (5)$$

where  $N$  is given by

$$N = \frac{\Delta H_v^2}{2 \cdot \Delta P \cdot \rho_l C_d^2 \left( \frac{1}{\rho_p} - \frac{1}{\rho_l} \right) T_s C_{pl}} + \frac{L_p}{0.1} L \quad (6)$$

where  $\Delta P$  = storage pressure - ambient pressure (Pa).

The above formulas overestimate the discharge rate, when it is occurring near the liquid surface in the container.

In the case of the discharge of pure liquids the Bernoulli equation is used

$$\dot{m} = C_d A \rho_1 \sqrt{2\Delta P / \rho_1 + 2gH} \quad (7)$$

where  $H$  = the liquid head (m) above discharge  
 $g$  = 9.81m/s<sup>2</sup>

For pressurised condensed gases a portion of the discharge will flash off immediately, this part  $F_v$  is calculated by using (8)

$$F_v = \frac{C_{pl}}{\Delta H_v} \cdot (T_s - T_{bp})N \quad (8)$$

where  $T_{bp}$  = the normal boiling point of the substance (K). Here it is assumed that the discharge is adiabatic.

### **Liquid pool formation and evaporation**

When a liquid or a liquefied gas is discharged a liquid pool can be formed. For gases liquefied by pressure a certain portion of the discharge is immediately flashed off. This fraction can be estimated using equation (8), however, experiments where pressure liquefied gases are discharged into free air have shown that this estimate is too low and often it is appropriate to assume that twice the value given by (8) is immediately vaporised. When the release is obstructed in some way by for instance a wall, then it is possible that a larger portion of the discharge forms a liquid pool. It is, however, very difficult to estimate how much enters the pool. If the discharge is obstructed, then FREIA assumes that it is escaping as a pure gas, from an area specified by the user, since this is assumed to be the worst case. Discharges that are pointing downwards are, however, treated as an evaporating pool. While for a discharge into free air it is assumed that no liquid pool is formed, instead they are treated as a jet, with a flash; this is what is usually observed when conducting experiments on pressure liquefied gases.

To estimate the evaporation rates two different situations must be considered. In one the discharge is of a liquefied gas, where the pool

temperature is equal to that of the normal boiling point of the exaporate, which is much lower than the ambient temperature. The other situation is where the temperature is equal to the ambient temperature and much lower than the boiling point of the substance. All calculations of evaporation rate are approximated to one of these models. However, the models may run into problems at low temperatures, i.e. at ambient temperatures below -40°C. In those instances it is recommended to execute the models from outside the package.

Evaporation model when  $T_{\text{source}} = T_{\text{bp}} \ll T_{\text{ambient}}$

For a discharge of a substance with a boiling point much lower than the surrounding temperature the Jensens model [3] is used. For these discharges the maximum possible evaporation rate equals the discharge rate. When there is a boundary present to prevent the pool spreading, the maximum possible evaporation rate is the minimum of the discharge rate and the rate when the pool area is equal to that of the boundary. The time  $t_d$  until the evaporation rate equals the discharge rate is given by

$$t_d = \frac{r_{\text{max}}^{4/3} \cdot (2\pi)^{1/3}}{(g \cdot \dot{V})^{1/3}} Q \quad (9)$$

where  $g = 9.81 \text{ m/s}^2$   
 $\dot{V} P =$  the volumetric discharge rate into the pool,  $\text{m}^3/\text{s}$   
 $r_{\text{max}} =$  the maximum radius of the pool is calculated from

$$r_{\text{max}} = \frac{\rho_l^{3/4} \dot{V}^{5/8}}{g^{1/8} s^{3/4}} \left(\frac{8}{3}\right)^{3/4} \cdot \frac{1}{\pi} \cdot \frac{1}{(2\pi)^{5/8}} Q \quad (10)$$

where  $\Delta_l =$  the liquid density,  $\text{kg/m}^3$

and  $s$  is given by

$$s = \frac{\Delta T}{\Delta H_v} \sqrt{\frac{\rho \lambda}{\pi}} c_{gr} R \quad (11)$$

where  $\Delta T = (T_{\text{source}} - T_{\text{ambient}})$ , K  
 $\Delta =$  ground density, typical value =  $2 \cdot 10^{-3} \text{ kg/m}^3$

- $c_{gr}$  = ground  $c_p$ , typical value 1000 J/kg/K
- $\delta$  = thermal conductivity of ground, typical value 1W/m/K
- $H_v$  = heat of vaporisation of release, J/kg

Of course in instances where there is a boundary present the radius calculated in (10) could simply be replaced by the radius of the boundary.

The maximum evaporation rate  $\dot{m}_{ev}$  is calculated from

$$\dot{m}_{ev} = \frac{s \cdot C \cdot \pi}{2} \cdot t_d T \quad (12)$$

with C given by

$$C = \frac{3}{4} \sqrt{2 \cdot \pi \cdot g \cdot \dot{V} U} \quad (13)$$

In cases where the duration of the discharge is shorter than  $t_d$ , then  $t_d$  in eq.13 is replaced by the duration of the discharge.

Evaporation model when  $T_{source} = T_{ambient} \ll T_{bp}$

At chemical sites the storage tanks often are surrounded by a wall, barrier or dike to decrease the pool area. If no boundary is present the liquid pool area is given by (14) regardless what type of soil the liquid pool is on.

$$A_p = 5.67 \cdot m^{0.492} V \quad (14)$$

- where  $A_p$  = liquid pool area,  $m^2$
- $m$  = amount of liquid released, kg

This formula is based on limited experimental data and is of course very crude [4]. This approximate model was chosen since very little is often known about the ground or soil where a release is occurring. In addition, slopes and holes in the ground makes it very difficult to predict pool spread.

To calculate the evaporation rate  $\dot{m}_{ev}$ , an experimentally well tested formula which correlates with the evaporation of hydrazine at temperatures above 0°C is used [4].

$$\dot{m}_{ev} = 1.046 \cdot 10^{-4} \cdot T_F \cdot \frac{P_s}{P_{sh}} M \cdot u^{0.75} W \quad (15)$$

where  $u$  = the wind speed, m/s  
 $P_s$  = the vapour pressure of the substance  
 $P_{sh}$  = vapour pressure of hydrazine from (16)  
 $M$  = the molecular weight  
 $T_F$  = a temperature correction factor from (17)

The vapour pressure of hydrazine  $P_{sh}$  is given by

$$\ln(P_{sh}) = 65.3319 - \frac{7245.2}{T} - 8.22 \ln(T) + 6.1557 \cdot 10^{-3} \cdot T X \quad (16)$$

where  $T$  = is temperature in degrees K and the pressure  $P_{sh}$  is in atmospheres.

$$T_F = 1 + 4.3 \cdot 10^{-3} \cdot T_p^2 Y \quad (17)$$

where  $T_p$  = is the temperature in degrees Celsius.

For discharges at an ambient temperature less than 0°C a model from Kanury [5] is used. This method is based on the dimensionless mass transport number  $B$ .

$$Y_{FW} = 1 / [1 + [p_a / p_F) - 1] \cdot (M_{air} / M_F)] Z \quad (18)$$

$$B = (Y_{F\infty} - Y_{FW}) / (Y_{FW} - Y_{FR}) AA \quad (19)$$

$$Re = u \cdot D / \nu BB \quad (20)$$

$$Nu = 0.037 \cdot Re^{0.8} \cdot Pr_{luft}^{1/3} CC \quad (21)$$

$$h = Nu \cdot k_{air} / DDD \quad (22)$$

$$\dot{m}_{ev} = A \cdot (h / C_{p,air}) \cdot \ln(1 + B)EE \quad (23)$$

where  $Y_{FW}$  = mass fraction fuel in gas phase at liquid surface  
 $p_a$  = air pressure  
 $p_F$  = vapour pressure of fuel  
 $M_{air}$  = molecular weight of air  
 $M_F$  = molecular weight of fuel  
 $Y_{F4}$  = mass fraction fuel in air above pool  
 $Y_{FR}$  = mass fraction fuel in pool  
 $Re$  = Reynolds number  
 $u$  = windspeed, m/s  
 $D$  = diameter of pool  
 $U$  = kinematic viscosity of air ( $15.08 \cdot 10^{-6} \text{ m}^2/\text{s}$ )  
 $Nu$  = Nusselt number  
 $h$  = convective heat transfer coefficient,  $\text{W}/\text{m}^2/\text{K}$   
 $k_{air}$  = conductivity of air ( $0.026 \text{ W}/\text{m}/\text{K}$ )  
 $\dot{m}_{ev} FF =$  mass loss from pool,  $\text{kg}/\text{s}$   
 $Pr_{luft}$  = Prandtl's number for air

For cases where the ambient and discharge temperatures are not equal, the averaged value is used. In the indoor scenario, the wind speed is assumed to be equal to 1 m/s.

### 3 Models used outside buildings

A description of the models used for evaluating the consequences of an accidental discharge outdoors is presented below. These are the models for dispersion, jet flame, pool fire, flash fire, UVCE, BLEVE and catastrophic tank failure.

#### **Dispersion**

For dispersal of gases outside buildings the dispersion model SLAB [6] is used. This model is based on concepts originally presented by Zeman [7]. SLAB handles four types of sources: a ground level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet and finally a ground based instantaneous release.

There are many different dispersion models available. However, the results from these compared with experimental studies differs widely. A comparison between some of the models and experiments is presented in [8], this showed that SLAB models the experimental results reasonably closely.

FREIA provides SLAB with the appropriate input data, executes the program and then extracts relevant data from the output provided by SLAB. For gaseous discharges the jet or instantaneous situations can be executed without any further calculation. If a gaseous discharge is obstructed, then it is assumed to be issuing in the gas phase from a new area provided by the user. For pure liquid discharges the input data are easily provided. The pool case utilises an evaporation rate and pool area which are calculated using equations 14-23. Unobstructed horizontal or vertical two-phase discharges are modelled as a jet, with a liquid fraction equal to 1 -2 times the flash, with the flash value given by eq. (8). Two phase discharges pointing downwards are treated as evaporating pools with the evaporation rate given by eqs. 9-13. Obstructed two phase discharges are treated as pure gaseous discharges issuing from a larger area than the area for calculating the discharge rate.

### **Jet flame**

To calculate the length  $L_f$  of a jet flame originating from a gaseous discharge, the following expression developed by Hawthorne, Weddel and Hottel [9] is used

$$L_f = d_o \cdot 5.3 / C_f \sqrt{\frac{T_f}{nT_i} (C_f + (1 - C_f) \cdot M_{air} / M_f) GG} \quad (24)$$

where  $n$  = is the ratio of the number of moles of reactants to moles of product for the stoichiometric mixture

$d_o$  = initial diameter of jet

$T_f$  = flame temperature, K

$T_i$  = initial temperature, K

$M_{air}$  = molecular weight of air (0.0288 kg/mole)

$M_f$  = molecular weight of fuel, kg/mole

$$C_f = (1 + r_i) / (1 + r) \quad (25)$$

where  $r_i$  = is initial air/fuel ratio  
 $r$  = stoichiometric air/fuel ratio

For the discharge of liquefied petroleum gas (propane) the jet flame length is obtained from [1] using equation (26)

$$L_f = 9.1 \cdot \sqrt{\dot{m}} \quad (26)$$

For discharges of other liquefied gases the jet flame length is given by eq. (27) from [10]

$$L_f = 18.5 \cdot \dot{m}^{0.4} \quad (27)$$

A spray fire may occur if the liquid discharges from an area smaller than  $0.000314 \text{ m}^2$  at a pressure greater than 30 bar. The length of this flame is calculated using eq. (28)

$$L_f = 0.075 \cdot (0.11 \cdot \Delta H_c \cdot v)^{0.6} \quad (28)$$

where  $v$  is the discharge velocity =  $\dot{m} / \rho_v / A$  (m/s).

To calculate the area of risk around a jet flame, the flame is divided into five point sources, each radiating at the power of 1/5 of the total radiative energy [11]. This is assumed to be 0.15 times the total energy released by methane flames and 0.30 times the total release from all other substances. Critical radiation levels of 35, 20 and 8 kW/m<sup>2</sup> were chosen, as these levels produce within 10 seconds third, second and first degree burns respectively on bare skin [12]. The same approach is used for evaluating the radiation level at a specific place.

### **Pool fire**

For calculations on pool fires the pool is assumed to ignite immediately on formation. For a continuous discharge this produces a maximum burning rate equal to the discharge rate, or equal to the mass loss rate per unit area for a pool of infinite diameter  $\dot{m}''_{\infty}$  times the area of the pool. For instantaneous releases it is equal to the latter. To estimate the radiation from

the fire the model of Mudan and Croce described below is used [13]. This takes into consideration flame tilt due to wind.

The flame height  $H$ , is calculated from a correlation developed by Thomas [14]

$$H / D = 42[\dot{m}'' / \rho_a \sqrt{gD}]^{0.61} \quad (29)$$

where  $\rho_a$  = is the density of air (1.293 kg/m<sup>3</sup>)  
 $\dot{m}''_{OO} =$  is the burning rate of pool, here assumed to be equal to  $\dot{m}''_{PP}$   
 $D$  = diameter of pool, m

The flame tilt  $\theta$  is calculated from

$$\cos \theta = \begin{cases} 1 & \text{for } u^* \leq 1 \\ 1 / \sqrt{u^*} & \text{for } u^* \geq 1 \end{cases} \quad (30)$$

where  $u^*$ , the nondimensional wind speed is given by

$$u^* = u / \left( \frac{g \dot{m}'' D}{\rho_a} \right)^{1/3} \quad (31)$$

where  $\Delta_a$  = the density of air at the appropriate temperature  
 $u$  = windspeed

The average emissive power  $E_{av}$  is estimated from

$$E_{av} = E_m e^{-S_e D} + E_s (-e^{-S_e D}) \quad (32)$$

where  $E_m$  = is the maximum emissive power of luminous spots (140 kW/m<sup>2</sup>)  
 $E_s$  = is emissive power of smoke (20 kW/m<sup>2</sup>)  
 $S_e$  = is a experimentally determined parameter (0.12 /m )

The radiation is given by

$$I = E_{av} \cdot \tau \cdot F_{max} \quad (33)$$

where  $\vartheta$  is the transmissivity given by

$$\tau = 1.11 \cdot x^{-0.09} UU \quad (34)$$

where  $x$  is the distance between the irradiated object or human and the centre of the pool fire.  $F_{\max}$  the maximum view factor is obtained from

$$F_{\max} = \sqrt{F_v^2 + F_h^2} \quad (35)$$

where  $F_v$  and  $F_h$  the vertical and horizontal view factors are given by

$$F_v = \frac{1}{\pi} \left( \begin{array}{l} \frac{a \cdot \cos \Theta}{b - a \cdot \sin \Theta} \cdot \frac{a^2 + (b+1)^2 - 2b(1 + a \cdot \sin \Theta)}{\sqrt{AB}} \\ \cdot \tan^{-1} \left( \sqrt{\frac{A}{B} \cdot \frac{b-1}{b+1}} \right) + \frac{\cos \Theta}{\sqrt{C}} \\ \cdot \left( \tan^{-1} \frac{ab - (b^2 - 1) \sin \Theta}{\sqrt{b^2 - 1} \sqrt{C}} + \tan^{-1} \frac{(b^2 - 1) \sin \Theta}{\sqrt{b^2 - 1} \sqrt{C}} \right) \\ - \frac{a \cdot \cos \Theta}{b - a \cdot \sin \Theta} \tan^{-1} \sqrt{\frac{b-1}{b+1}} \end{array} \right) \quad (36)$$

$$F_h = \frac{1}{\pi} \left( \begin{array}{l} \tan^{-1} \sqrt{\frac{b+1}{b-1}} - \frac{a^2 + (b+1)^2 - 2(b+1 + ab \cdot \sin \Theta)}{\sqrt{AB}} \\ \cdot \tan^{-1} \sqrt{\frac{A}{B} \cdot \frac{b-1}{b+1}} + \frac{\sin \Theta}{\sqrt{C}} \\ \cdot \left[ \tan^{-1} \frac{ab - (b^2 - 1) \sin \Theta}{\sqrt{b^2 - 1} \sqrt{C}} + \tan^{-1} \frac{(b^2 - 1)^{0.5} \sin \Theta}{\sqrt{C}} \right] \end{array} \right) \quad (37)$$

where  $a$  is the ratio between the flame height and radius,  $b$  is the ratio between the observer distance and the flame radius and  $A, B, C$  is given by

$$\begin{aligned} A &= a^2 + (b+1)^2 - 2a(b+1) \sin \Theta \\ B &= a^2 + (b-1)^2 - 2a(b-1) \sin \Theta \\ C &= 1 + (b^2 - 1) \cos^2 \Theta \end{aligned} \quad (38)$$

Hazardous radiation levels of 5.0 kW/m<sup>2</sup> and 2.5 kW/m<sup>2</sup> were chosen, the pain threshold is reached in 15 s with 5.0 kW/m<sup>2</sup> exposure. To estimate the radiation received at a certain point the same approach was used.

### Flash fire

In the flash fire case the ignited cloud is assumed to be formed as a half ellipsoid [16], with the length and width taken from the data obtained from SLAB. The cloud is assumed to expand to eight times its initial volume upon ignition. The radiation from this half ellipsoid is assumed to be from five point sources as in the jet flame scenario. The total emissive radiation  $q_e$  is:

$$q_e = A_f \cdot \sigma \cdot (\epsilon_g T_g^4 - \epsilon_g T_a^4) \quad (39)$$

where  $\Phi$  = is the Stefan Boltzmann constant ( $5.76 \cdot 10^{-8} \text{ W/m}^2\text{K}^4$ )  
 $\epsilon$  = is the emissivity of hot gas, here taken as 1.0  
 $A_f$  = flame area, m<sup>2</sup>

If  $q_e$  is assumed to be equal to the cooling of the hot gas  $q_{\text{loss}}$ , the duration of the flash fire  $t_{\text{eff}}$  and the average radiation temperature  $T_{g \text{ av}}$  can be estimated as follows:

$$q_{\text{loss}} = c_{p,\text{air}} \cdot \rho_g \cdot V_f \cdot dT_g / dt \quad (40)$$

$$t_{\text{eff}} = 3t_{1/2} \quad (41)$$

$$t_{1/2} = \frac{1}{2kT_a^3} \left[ \tan^{-1} \left( \frac{\alpha+1}{2} \right) - \tan^{-1} \alpha - \frac{1}{2} \ln \left( \frac{\alpha+1}{\alpha+3} \right) \right] \quad (42)$$

$$T_{g \text{ av}} = (T_{gi} + T_a) / 2 \quad (43)$$

$$\beta = T_{gi} / T_a \quad (44)$$

$$k = \frac{A_f \sigma}{C_p \rho V_f} \quad (45)$$

where  $\rho_g$  = density of hot gas layer ( $\rho_{air}$ ), kg/m<sup>3</sup>  
 $V_f$  = volume of flash fire. m<sup>3</sup>  
 $T_g$  = gas temperature, K  
 $t_{eff}$  = effective duration of flash fire, s  
 $T_{1/2}$  = half-life of flash fire, s  
 $A_f$  = flame area, m<sup>2</sup>  
 $T_{gi}$  = initial gas temperature K, assumed to be equal to the adiabatic flame temperature.

When estimating the radiation flux at a certain point the same approach is used. The model described above by Eisenberg et al. [15] has severe limitations, but is presently the only appropriate one available.

## UVCE

To estimate the pressure effects from an Unconfined Vapour Cloud Explosion (UVCE) the TNT model is used [1]. The energy contained in the flammable cloud is converted into an equivalent mass TNT and this is then compared with the pressure developed by a TNT explosion. The explosive effect due to a TNT charge is well documented, and is often in the form of curves covering several explosion parameters, such as pressure and impulse power. The equivalent mass of TNT,  $W$  is given by

$$W = \frac{m \cdot E_c \cdot \eta}{E_{cTNT}} \text{DDD} \quad (46)$$

where  $\eta$  = is an empirical explosion factor [ 0.01 - 0.1] here assumed to equal 0.1  
 $m$  = is mass of flammable gas, kg  
 $E_c$  = is heat of combustion of gas, kJ/kg  
 $E_{cTNT}$  = is heat of combustion of TNT, ( 4450 kJ/kg)

The TNT model is often used to estimate pressure effects due to UVCE. A selection of various types of damage caused by explosive overpressures is presented in Table 2. However, the model is not valid within the cloud since it is approximated to a small volume of TNT.

Table 2. Damage due to explosive overpressure.

Overpressure, Pa	Damage
6900	Partial demolition of houses
16500	1% eardrum rupture
84 000	90% eardrum rupture
41 000	Nearly complete destruction of houses
69 000	Probable total building destruction
107 000	1% Fatalities due to direct blast
200 000	99% Fatalities due to direct blast

## **BLEVE**

For the BLEVE (Boiling Liquid Expanding Vapor Explosion) scenario the diameter  $D_B$  of the BLEVE is given by the following equations from [1]

$$D_B = 6.48 \cdot m^{0.325} EEE \quad (47)$$

and  $m$  = released mass, kg

The duration  $t_B$  is given by

$$t_B = 0.825 \cdot m^{0.26} FFF \quad (48)$$

and the height  $H_B$  above ground is given by

$$H_B = 0.75 \cdot D_B GGG \quad (49)$$

All available models for estimating the consequences of a BLEVE are very similar, some variations in the constant in eqs. 47 to 49 do however exist.

The BLEVE is assumed to radiate as a point source. The dangerous radiation levels are chosen dependant on the duration of the event. For those less than 1.0 s the chosen levels are 50, 120 and 200 J/m<sup>2</sup> as these cause first, second and third degree burns respectively. For durations longer than 15 seconds the radiation levels are chosen as 80, 200 and 350 J/m<sup>2</sup> as these also cause first, second and third degree burns respectively. Intermediate injury levels are obtained by interpolation.

The number of fragments formed in an explosion can be calculated and also the distance they travel. The number of fragments  $n_r$ , are obtained from the empirical formula

$$n_r = -3.77 + 0.0086 \cdot V_{\text{vessel}} \text{HHH} \quad (50)$$

where  $V_{\text{vessel}}$  = the volume of the vessel,  $\text{m}^3$

this is valid for vessels with a volume in the range  $700\text{-}2500 \text{ m}^3$ . By assuming that all fragments are equal of size, the weight and area of each can be calculated by assuming the vessel is a sphere. The initial velocity  $U_0$  is the given by

$$U_0 = 2.05 \cdot (P_b \cdot d^3 / W_f)^{0.5} \text{III} \quad (51)$$

- where  $P_b$  = rupture pressure, psig
- $d$  = fragment diameter, inches
- $W_f$  = weight of fragments, lb
- $U_0$  = initial velocity, ft/s

The distance travelled by the fragments are obtained from figure 3 assuming a drag coefficient  $C_D$  of 0.47.

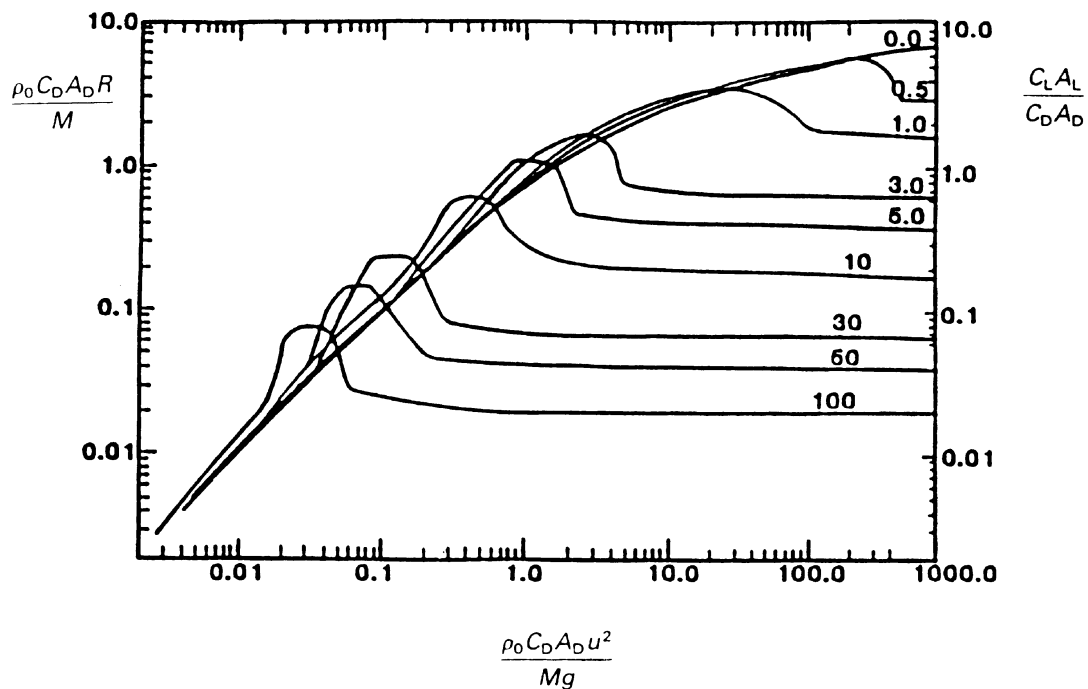


Figure 3. Distance travelled by flying fragments [1].

### **Catastrophic tank failure**

In the cause of a catastrophic tank failure, the impact of flying fragments is calculated as described above for the BLEVE. The expansion of the gas is transformed to an equivalent amount of TNT,  $W$  and as in the UVCE case, the damage is estimated from curves [1]. The equivalent amount of TNT,  $W$  is given by

$$W = 1.4 \times 10^{-6} V_g [p_i / p_a] [T_0 / T_1] R_R T_1 \ln [p_i / p_f] \text{ JJJ} \quad (52)$$

where  $W$  = energy in lb TNT  
 $V$  = volume of compressed gas, ft<sup>3</sup>  
 $p_i$  = initial pressure of compressed gas  
 $p_f$  = final pressure of expanded gas  
 $p_a$  = ambient pressure  
 $T_1$  = temperature of compressed gas, °R  
 $T_0$  = standard temperature, 492°R  
 $R_R$  = gas constant, 1.987 Btu/ lb mol/°R KKK  
 $1.4 \times 10^{-6}$  = conversion factor (this factor assumes that 2000 Btu = 1 lb TNT)

When the actual burst pressure is unknown it is assumed to be four times the design pressure.

### **4 Models used inside buildings**

The models for the dispersion and the general consequences of a fire, etc. inside buildings are somewhat different from the outdoor scenario. A description of the various models used for estimating the overpressure created in the room due to the discharge, the jet-dispersion, the concentration build up a confined space, the jet flame, the pool fire and the explosion is presented below.

### Physical explosion

When a large discharge is occurring inside a building the pressure build-up may be strong enough to break a door or window. In houses, doors and windows start breaking at an overpressure of 30 mbar. The pressure in the room is calculated by assuming that the volumetric flow of gas and air from the room,  $V_{out}$  is given by

$$V_{out} = 0.6 \cdot A_o \cdot (2 \cdot \Delta P / 1.2)^{0.5} LLL \quad (53)$$

and thus the overpressure  $\Delta P$  is given by

$$\Delta P = (V_{in} - V_{out}) / V \cdot 1000 MMM \quad (54)$$

where  $V_{in}$  = the amount of gas flowing into room

$V$  = volume of room

$\Delta P$  = overpressure, Pa

$A_o$  = area of openings,  $m^2$

In the instantaneous case the discharge is assumed to last for 1 second.

### Jet dispersion

For a jet dispersion inside a building the formula developed by Chen and Rodi [17] is used. This formula is valid for Froude numbers  $Fr$ , less than 30000.

$$\frac{\overline{C_{xr}}}{C_o} = 5 \cdot \sqrt{\rho_a / \rho_g} \cdot d_o / x \exp(-57.3 \cdot r^2 / x^2) NNN \quad (55)$$

$$Fr = \frac{U_o^2 \rho_o}{gd_o(\rho_a - \rho_g)} OOO \quad (56)$$

where  $\overline{C_{xr}}$  PPP = average concentration at (x,r)

$C_o$  = initial concentration often (100%)

$\Delta_a$  = air density,  $kg/m^3$

$\Delta_g$  = gas density,  $kg/m^3$

$d_o$  = discharge diameter, m

$U_o$  = initial velocity of gas, m/s

## Concentration Build-up

In most practical scenarios concerning events inside buildings there are enough obstacles to produce what is termed a "well-stirred reactor". When calculating the concentration this assumption is therefore made and is given by eq. 57 from [18].

$$C = \frac{100 Q_g}{Q_a + Q_g} \left[ 1 - \exp \left( -(Q_a + Q_g)t / V^* \right) \right] \quad (57)$$

where  $Q_g$  = is volumetric flow of gas into room, m<sup>3</sup>/h or m<sup>3</sup>/s  
 $Q_a$  = is volumetric ventilation rate, m<sup>3</sup>/h or m<sup>3</sup>/s

$V^*$  is chosen as the volume of heavy gas beneath a downward discharge, with the ventilation in the same downward direction. For those buoyant gas discharges which are directed upwards, with the ventilation in the same direction,  $V^*$  is taken as the volume of the room above the discharge. In all other cases  $V^*$  is equal to the room volume. For flammable substances the time at which the concentration exceeds ¼ of the lower flammability limit is calculated. For non-flammable discharges a concentration level of interest to the user is chosen.

Another quantity of interest is the decrease in the temperature in the room due to the discharge. An estimate of this is obtained by calculating the equivalent volume of air which is involved in the temperature decrease to the boiling point, this is given by:

$$V_{\text{cold}} = \frac{m_{\text{ev}} \cdot \Delta H_v}{C_{p,\text{air}} \rho_a \Delta T} \quad (58)$$

where  $m_{\text{ev}}$  = total evaporated mass, kg  
 $C_{p,\text{air}}$  =  $C_p$  of air, J/kg/T  
 $\Delta H_v$  = heat of vaporisation, J/kg  
 $\Delta T$  =  $T_s - T_{\text{bp}}$ , K  
 $\Delta_a$  =  $\Delta$  of air at  $T_{\text{av}}$ , kg/m<sup>3</sup>  
 $T_{\text{av}} = \frac{T_s + T_a}{2}$ , K  
 $T_s$  = storage temperature, K

(59)SSS

$T_a$  = ambient temperature, K

### **Jet flame**

In the case of a jet flame the fire scenario section of the program is consulted. A RHR curve is created by assuming that the rate of heat release increases linearly from zero to the maximum in 10 seconds. This maximum is equal to the discharge rate  $\dot{m}$  times the heat of combustion  $H_c$ . The radiation flux from the jet flame to the components can be calculated; two basic types can be considered, point or linear (pipes and cables). For point components the radiation is calculated as in the exterior scenario. For linear ones, the radiation is calculated at a point where the radiation is at a maximum. The highest possible radiation flux is taken as 200 kW/m<sup>2</sup>, which occurs when the component is in contact with the flame. The radiation flux is added to that from the gas layer.

### **Pool fire**

For pool fires inside buildings a RHR curve is created by FREIA and the fire scenario is then initiated.

### **Explosions inside buildings**

The over pressure in a confined explosion is due to the expansion of the hot gases. There is often some kind of explosion vent, which can even be a door or a window. When the explosion vent is released a second pressure peak is produced by the turbulence created, as presented in figure 4 below. To estimate the over pressure developed during explosions inside buildings the Cabbage and Simmonds model [18] is used

$$p_1 = S_0(4.3KW_e + 28) / V^{1/3} TTT \quad (60)$$

$$p_2 = 58\beta S_0 K UUU \quad (61)$$

$$K = A_s / A_v \text{ when vent is on large surface VVV} \quad (62)$$

$$K = V^{2/3} / A_v \text{ otherwise WWW} \quad (63)$$

where  $p_1$  = first pressure peak, mbar  
 $p_2$  = second pressure peak, mbar  
 $K$  = vent coefficient  
 $W$  = weight per unit area of vent cladding,  $\text{kg/m}^2$   
 $V$  = room volume,  $\text{m}^3$   
 $\Xi$  = turbulence factor  
 $A_v$  = vent area,  $\text{m}^2$   
 $A_s$  = area on which vent is placed,  $\text{m}^2$

This model is valid if  $K < 5$   $W < 24$  and  $L_{\text{max}}/L_{\text{min}} \# 3$ , with  $L_{\text{max}}$  being the maximum dimension of the room and  $L_{\text{min}}$  the minimum.

An explosion is possible if the maximum concentration in the room exceeds 1/4 of the Lower Flammability Limit.

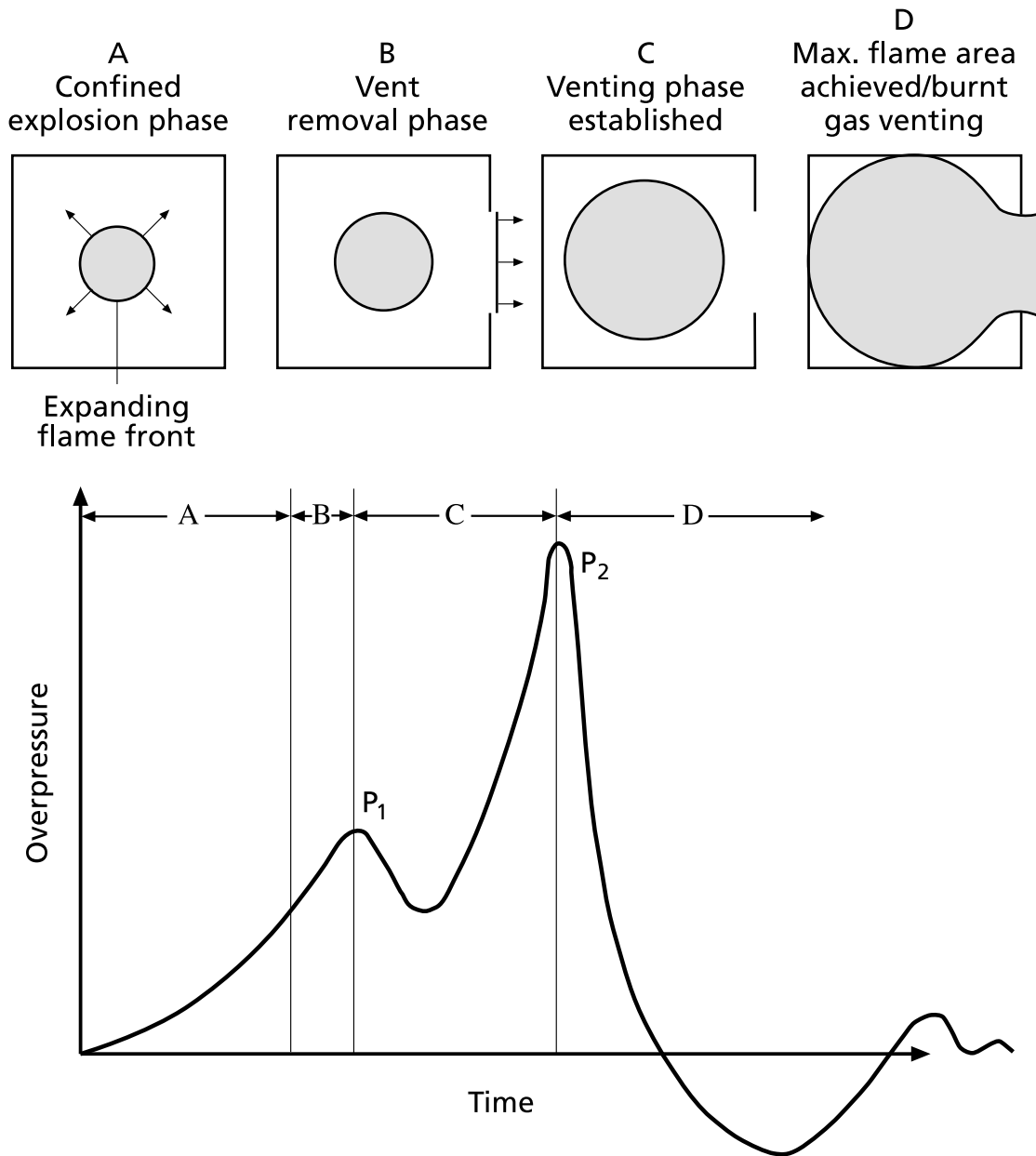


Figure 4. Pressure peak of an explosion inside a building [18].

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## Appendix B

### Auxiliary Databases Included in the FREIA Package



## Auxiliary Databases Included in the FREIA Package

Included in the FREIA package are databases for building materials, fire response, physical data of gases and liquids, the fire characteristics of liquid and solid materials, damage criteria of components and also one database, with statistical data on accidental discharges and ignition. All these databases can be edited by the user. A short description of these is presented below.

### Database for building elements

CATEDIT is a database for the elements used in buildings (walls, floors, etc.). The routine is taken directly from the FPETool program package developed at NIST. The properties stored are thermal conductivity ( $k$ ), specific heat ( $C_p$ ), density ( $\rho$ ) and emissivity ( $\epsilon$ ). The user can change any of the values and add or delete material. The database can be accessed by the simulation programs but changes can only be made permanent by using the CATEDIT routine.

### Database for solid fuels

SOLEDIT is a database for the combustion properties of solid fuels. Three are included, namely the effective heat of combustion ( $h_e$ ), energy release rate per projected fuel area ( $q''$ ) and the fire growth rate ( $a$ ). The data originates from Babrauskas [1] and Ondrus [2]. The database can be accessed by the auxiliary program EFFECT, but again changes to the database can only be made permanent by using the SOLEDIT routine.

### Database for liquid fuels

LIQEDIT is a database for the combustion properties of liquid fuels. The four included are the effective heat of combustion ( $h_e$ ), density ( $\rho$ ), mass loss rate per unit area for large spill areas ( $\dot{m}''_{\infty}$ ) and the K value (this is the product of the extinction-absorption coefficient ( $K$ ) and the mean beam length corrector ( $L$ )). The data originates from Babrauskas [1] and Ondrus [2]. As for SOLEDIT this database can be accessed by the auxiliary program

EFFECT, but changes to the database can only be made permanent by using the LIQEDIT routine.

Program EFFECT: assists in creating the heat release rate curve

This program allows the user to access the SOLEDIT or LIQEDIT databases, or to simply specify the required parameters, without using the databases. The routine assumes that there are three phases of fire development; a growth phase, a steady state phase and finally a decay phase.

When using the SOLEDIT database, information on the growth rate constant is presented and the fire is assumed to grow according to the equation

$$q = at^n A \quad (1)$$

where  $q$  = Rate of heat release (kW)  
 $a$  = A constant (suggested values are included in the routine)  
 $t$  = Time since initiation (s)  
 $n$  = An exponent (usually 2, in which case the fire is referred to as a  $t^2$  fire)

The user can also specify an exponential growth curve, given by

$$q = Be^{bt} B \quad (2)$$

where  $q$  = Rate of heat release (kW)  
 $B$  = Constant (In EFFECT "B" is set at 1kW)  
 $e$  = e (the base of natural logarithms)  
 $b$  = A constant (the suggested values are included in the routine)  
 $t$  = Time since initiation (s)

If there is a limited amount of fuel available, the fire will only grow to a certain maximum heat release rate,  $q_{\max}$ . The database supplies a value for the material heat release rate per projected floor area. The user can prescribe a certain floor area and thus  $q_{\max}$  can be calculated as

$$\dot{q}_{\max} = \dot{q}'' A_f C \quad (3)$$

where  $\dot{q}''$  = the material heat release rate per projected floor area

$A_f$  = the projected floor area of fuel

In order to specify the duration of the steady state phase the user must either assume a certain duration, or present as the input, the mass of material which will burn during the growth and steady state phases. By inputting the effective heat of combustion (from the database), the mass loss rate can be calculated and the duration  $t_2$  is then obtained by integrating the mass loss rate from  $t = 0$  to  $t = t_2$ .

A similar procedure is followed when using the database for liquid fuels. The growth is calculated using equation (1) where the growth constant  $a$  is assumed to be  $0.1876 \text{ kW/s}^2$  (corresponding to an ultra-fast growth rate). The user can change this value.

In order to estimate the maximum heat release rate  $\dot{q}_{\max}$ , the user must specify a certain quantity of liquid  $L$ , in litres. The thickness of the liquid spill ... is assumed initially to be 3 mm. This value can be changed by the user.

This allows the area of spill to be calculated from

$$A_f = L / (1000 \delta) D \quad (4)$$

With the above data the mass loss rate is calculated from [1]

$$\dot{m}'' = \dot{m}''_{\infty} (1 - e^{-DK\beta}) E \quad (5)$$

where  $D$  is the spill diameter.

The maximum heat release rate is then calculated from [1]

$$\dot{q}_{\max} = \dot{m}'' \cdot \Delta H_e \cdot A_f F \quad (6)$$

The duration of the growth and the steady state phases is calculated by integration, as above.

The decay phase of the fire can be specified as following a power law, or an exponential decay. This is carried out by a similar but reversed procedure to that described for the growth phase.

## Program INTOOL: helps to create an input file

INTOOL was originally a part of the FPETOOOL package, but changes have been made so that the program fits into the FREIA package. This program asks questions on room geometry as well as all the other required input data. No calculations are performed in this program.

## PHYSDATA: a database for physical data

The database PHYSDATA contains up to 20 entries depending on whether the substance is flammable or not, these entries are:

### for all kinds of substances

name	each substance can have up to five different names
A,B,C	vapour pressure constants
flammable	Y/N
M	molecular weight, kg/mole
heatvap	Heat of vaporisation, J/kg
TBP	Normal boiling point, K
cp <sub>g</sub>	C <sub>p</sub> for the gas phase, J/kg/K
cp <sub>l</sub>	C <sub>p</sub> for the liquid phase, J/kg/K
liqdens	Density in liquid phase, kg/m <sup>3</sup>
gamma	Specific heats ratio
gasdens	Density in gas phase, kg/m <sup>3</sup>

### for flammable substances

heatcomb	Heat of combustion, MJ/kg
LFL	Lower Flammability Limit
UFL	Upper Flammability Limit
lamburn	Laminar burning velocity, m/s
n	Ratio of moles reactants to moles products for stoichiometric reaction.
r	Stoichiometric air/fuel ratio
cf	=1/(1+r)
tf	Adiabatic flame temperature, K
flashpoint	Flashpoint of liquid, K

## STATIST: a database of statistical information

This database contains statistical information on initial events. It is not directly used by the package, but is provided as an aid for the user to decide on what initial event should be chosen. The entries are: name of the component, component type, media, dimensions, failure mode, frequency function, frequency of event, upper confidence level, lower confidence level and reference information. Input is optional on all entries except for the frequency.

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