

# Airborne releases from fires involving chemical waste—a multidisciplinary case study

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## Abstract

A multidisciplinary study of fires in chemical waste at a Danish chemical company has been carried out in order to estimate the concentrations of combustion products in the surroundings. The first part of the study addressed the characterisation of the waste and the assessment of fire cases which formed the basis for the experimental work and determination of fire effluents. The combustion experiments were carried out using a tubular furnace, following DIN 53436. Secondly, the source term concentrations were estimated, and calculations of plume rise and dispersion of combustion products in the surroundings were performed. Finally, an uncertainty assessment has been carried out for each part of the study. For some of the issues the uncertainties are described qualitatively and for others the uncertainties are expressed quantitatively. © 1998 Elsevier Science B.V.

*Keywords:* Chemical fires; Combustion; Consequence assessment

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## 1. Introduction

The paper presents the approach used and the results of a consequence assessment study of fires involving chemical waste at a Danish chemical company [1]. The analysis was carried out in 1996 by request from the Danish Environmental Protection Agency (EPA) and the project was followed by an advisory committee with members from: the Danish EPA, the fire brigade, the county board and the municipality.

The study focused on airborne releases comprising: (a) determination of the combustion products and the source term concentrations; and (b) assessment of plume rise and

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the concentration of combustion products in the surroundings as function of distance from the source. It is stressed, that toxicological and ecotoxicological assessments were not included in the consequence assessment. The toxicological assessment has been carried out afterwards by the Danish EPA.

The objective of this paper is two-fold: (a) to describe and discuss the advantages and limitations of the applied approach for assessment airborne releases from fires involving chemical waste; and (b) to present the results of the study together with an assessment of uncertainties.

## 2. Approach

The chemical waste types in question can be characterised as unique mixtures of chemicals with lacking data on combustion properties and characteristics which implied that information concerning fire conditions and source term characteristics not were available. Therefore, the approach for the study was carefully discussed, and it was decided to carry out the following steps:

- inspection and description of the site
- categorisation of waste types and collection of samples at the plant
- assessment of fire cases
- combustion experiments
- assessment of source term concentrations from real fires
- assessment of the plume rise and dispersion calculations
- assessment of uncertainties.

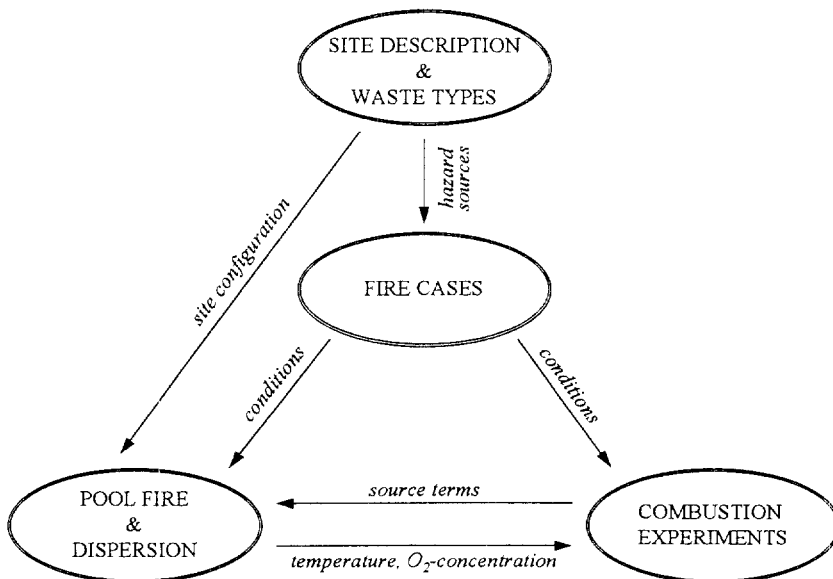


Fig. 1. Approach for assessment of airborne releases from fires involving chemical waste.

Going from one step of the study to the next implies application of different analysis techniques or methods, and an essential aspect has been to consider in detail the links between the different steps in order to ensure that the output (conditions, results, data, etc.) obtained in one step was a usable and adequate input to the subsequent step. Carrying out an analysis of this kind is not a straightforward process, and at each step the conditions and the results from the previous steps have been discussed and evaluated more than once. Therefore, the links between the different issues are of both retrospective and progressive character. The approach of the study is illustrated in Fig. 1. In this paper, the focus is on the lessons learned in linking the results from the single steps together and less emphasis will be laid on the techniques and methodologies used in each step. These are described in the open literature and references are recommended.

### 3. Site description

The company is a small enterprise (about 75 employees) producing fine chemicals and intermediates for the chemical and pharmaceutical industry (fungicides, preservatives, etc.). The site consists of facilities for production, laboratory, transport, waste water treatment and storage (raw materials, products, waste), see Fig. 2. The company is located in a small village with residences and a highway close to the plant.

The chemical waste is situated close to a pilot laboratory building and separated from the production units. The shortest distance between the waste storage and the production

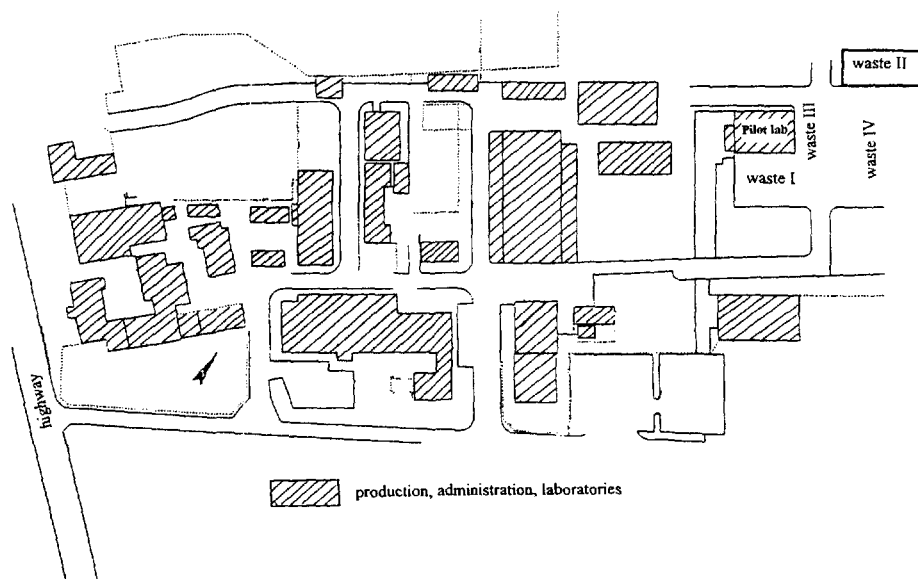


Fig. 2. Site plan.

facilities is about 35–40 m and the distance to neighbours and the highway is about 150–200 m. The chemical waste is placed in the open air in drums, tanks, etc. At the time of inspection the amount of chemical waste stored at the site was about 1500–1600 ton.

#### **4. Categorisation of waste types and collection of samples at the plant**

The chemical waste can be divided into four categories: Waste I, II, III, and IV.

Waste I (about 500 ton) consists of distillation residues from benzylcyanide synthesis and is stored in an open concrete storage tank of 12 m by 18 m covered with canvas. It is a solid under ambient conditions, with a melting point between 50°C and 80°C. Its composition is not fully known, it may contain a substantial amount of polymers. It is assumed to consist of benzylcyanide (5%), benzylphenylacetate (6%), phenylacetamide (15%), benzylcyanide (19%) tribenzylamine (17%), phenylacetylbenzylcyanide (25%) and ammonium salts. The estimated heat of combustion (33 MJ/kg) agrees very well with provided data (32–33 MJ/kg). If no specific data could be found, data for heavy or crude oil has been used (which has heat of combustion between 39 and 43 MJ/kg).

Waste II (about 250 ton) is stored in two 200 m<sup>3</sup> storage tanks in a tank pit and is a mixture of benzylalcohol, benzylcyanide, benzylchloride and phenylacetamide. The flash point of benzylchloride is 67°C, so the contents of the tanks can be ignited easily (but under ambient conditions the vapour in the tank would not be explosive).

Waste III (about 250 ton) is a distillation residue stored in drums. The composition of waste III varies but the content can be indicated as follows: antranillic acid (about 1%), benzoic acid (about 11%), monothiosalicylic acid (about 6%), dithiosalicylic acid (about 5%), trithiosalicylic acid (about 3%), ashes (about 14%) and water (about 60%). The combustion experiments confirmed a larger than usual amount of water in the samples. The high water content lowers the net combustion heat considerably and makes it difficult to ignite.

Waste IV (about 500–600 ton) can be characterised as ‘other chemical waste’. This category contains among other things chemical waste with a large content of solvents, e.g. ethanol and toluene.

Samples for combustion and thermographic experiments were taken from each of the four waste categories. For waste I, one sample was taken from the surface and one sample from a depth of about 75 cm. Waste II is stored in two storage tanks and one sample was taken from the middle of each tank. Waste III is stored in drums and samples were taken from the surface of two drums randomly chosen. From waste IV ‘other chemical waste,’ one sample was taken from a drum containing a homogeneous mixture of ethanol and toluene.

Waste I, II and III are all inhomogeneous mixtures of chemicals for which many of the necessary physical and chemical data have not been available. Consequently, an essential source to uncertainty is related to the used data, which have been estimated from the experimental work, information from the company and data from the open literature.

## 5. Assessment of fire cases

Much attention has been laid on the development of fire cases. The fire cases should cover realistic fires, ranges of toxic material production rates, and ranges of plume rise. Toxic material production rates depend on the combustion conditions (temperature and oxygen supply) and plume rise on the size and heat release of the fire. We decided to define two fire cases for each type of waste: (a) A relatively small fire, which can be considered to be a starting fire at relatively low temperature and little plume rise. Additionally, low ventilation conditions have been chosen as a larger fraction of potentially harmful organic combustion products is expected compared to well ventilated conditions. (b) A fully developed fire, involving the majority of the inventory of the waste on the site, with high temperatures, sufficient ventilation and large plume rise.

The fire cases have been simulated by applying the model fire classification according to the ISO standard [2,3]. However, a fire might change character over time, thus one model fire is not enough to predict real fires [4]. On the basis of this classification three different fire conditions are considered: (a) Fire condition A (900°C furnace temperature and air ventilation with 21% oxygen) to simulate a fully developed fire under optimal oxygen supply. (b) Fire condition B (900°C furnace temperature and air ventilation with 5% oxygen) to simulate a fully developed fire under reduced oxygen supply. (c) Fire condition C (500°C furnace temperature and air ventilation with 5% oxygen) to simulate the oxidative/pyrolytic decomposition phase of a fire.

It is assumed that condition A mainly simulates the chemical processes which are on-going in the flaming zone (mostly the outer part of the flame), whereas condition B mainly simulates the chemical processes which are on-going in the core of the flame, where the non-flaming pyrolysis and oxidising processes happen.

The conditions in the tubular furnace are described by laminar flows and almost complete combustion under A and decreasing combustion efficiency from B to C. As a rough estimate, it is further assumed that the real flaming conditions for the fully developed fires are in between conditions A and B and that the starting fire conditions are in between condition C and B.

The waste I initiating fire is thought to involve an area of 4 m<sup>2</sup>. The fully developed fire is assumed to involve a pool fire at the full size of the container (12 × 18 m). This case is characterised by an enormous heat release (in total 364 MW) and plume rise, not influenced by the buildings.

It is assumed that a waste II fire can start within the horizontal tank with one manhole (or comparable size opening) open, with a diameter of 1 m. The rate of combustion is supposed to be dominated by the maximum ventilation flow rate through the hole. This ventilation rate is estimated to be about 0.3 kg/s air, leading to a combustion rate between 0.02 and 0.03 kg/s. One might question whether a fire under the above conditions can exist. It will probably be very unstable. Condition C was chosen to simulate the fire. If one of the tanks fails, the contents will remain in the basin below the tanks. The basin has a dimension of 8.3 m wide and 25 m long. A pool fire of this size will develop rapidly.

Three fire cases have been considered for waste III. The initiating fire is considered to be a kind of decomposition and it is assumed that only one drum will be involved.

Due to the water content the flame temperature will be low (500–600°C). Condition C is used to simulate the fire. It is assumed that the (plastic) drums will fail. Waste III will melt and form a pool of an principle unknown size. The pool size has been estimated to cover the storage area, i.e. 8 m × 12 m. The combustion rate is estimated to be about 0.3 kg/s. Due to the water content the flame temperature will be low. The heat release is also limited (1.6 MW), therefore only condition C was assumed to be relevant in this case. Due to the very high water content a self drying mechanism resulting in a slowly increasing heat release is not considered. If waste III is involved in a larger fire (e.g. engulfment from burning drums with solvent like waste IV) the temperature in the fire may be larger than if waste III burns on its own. With the same pool area as for an unsupported fire (see above), this will lead to a combustion rate of about 5 kg/s. The flame temperature is assumed to be high. It is assumed that water evaporates prior to ignition and therefore conditions A and B have been chosen to simulate the third fire case.

Most drums of waste IV contain a homogeneous mixture of ethanol and toluene. As initiating event we assume a fully developed pool fire of the size of a single (steel) drum. The combustion rate will be 0.07 kg/s. For the fully developed case it is assumed that the (steel) drums will fail. The flammable liquid will pour out and form a pool of unknown size. The pool can fill the whole storage and road up to the drains in the road. This area is estimated as 20 × 30 m. Rates of combustion are then estimated to be almost 40 kg/s. For waste IV no experimental simulation was performed as the fire behaviour is assumed to be that of toluene and ethanol leading to high temperatures and combustion products like CO, H<sub>2</sub>O and CO<sub>2</sub>.

The development of fire cases was a key element of the study and the links to the combustion experiments and the consequence calculations were of retrospective character. The fire cases were prepared on basis of site inspection and considerations concerning release of chemicals and the possible pool sizes. The coverage of study was ensured by setting up two fire cases for each waste category: a relatively small fire which can be considered to be a starting fire, and a fully developed fire involving the majority of the inventory of the waste on the site.

## 6. Combustion experiments

### 6.1. Experimental setup

Combustion experiments have been carried out using a tubular furnace after DIN 53436. The furnace is designed to simulate steady state conditions, e.g. non-flaming oxidative and pyrolytic conditions and fully developed fires according to the ISO classification. The furnace has been slightly modified in order to ensure a constant production of combustion gases [5,6]. Also in a recent project the results obtained in the tubular furnace have been compared with larger scale experiments, which were in reasonable agreement for a number of combustion products [7,8]. The DIN 53436 furnace (see Fig. 3) consists of a quartz combustion tube (length 1 m, diameter 4 cm) and a movable (1 cm/min) annular electric oven enclosing a section of the tube.

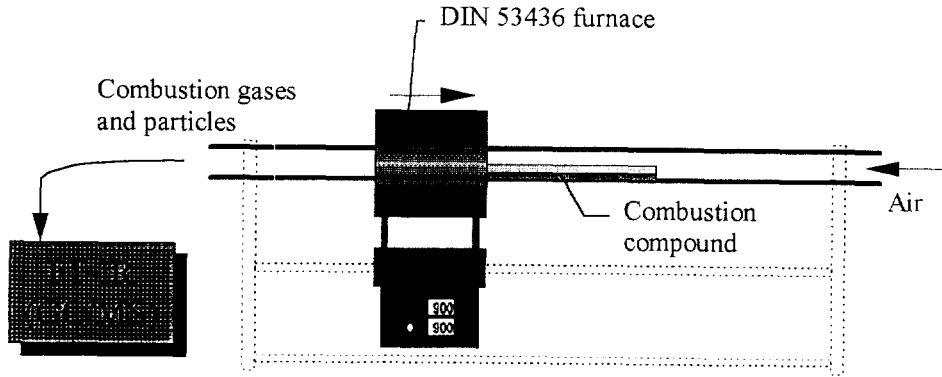


Fig. 3. Setup of the DIN 53436 furnace.

The sample (1–3 g) is placed in 24 small vessels posed in a 40-cm quartz boat. Air streams through the quartz tube during the experiment and transports the combustion products into the FTIR equipment. A Bomem MB100 FTIR instrument was used for on-line gas analyses in the DIN 53436 experiments. The instrument was equipped with a multiple-pass gas cell of pathlength 6.4 m and volume 0.7 l. The sample line and the gas cell were heated to 180°C in order to avoid combustion gas condensation.

The combustion experiments carried out during the study can be characterised as screening experiments indicating that the experimental conditions do not represent all situations which can appear during a fire course.

### 6.2. Determination of fire effluents and source terms

In Table 1 some important combustion products are presented for the four categories of chemical waste. A key point of the study was to determine the amount of cyanides in

Table 1  
Combustion products

Waste type	Condition A: Fully developed fire at optimal oxygen supply	Condition B: Fully developed fire at reduced oxygen supply	Condition C: Fire at non-flammable oxidative conditions
Waste I	e.g., CO, NO, HCl and N <sub>2</sub> O	HCN, acetylene, methane, and aromatic compounds	Many different organic compounds
Waste II	e.g., CO, NO, N <sub>2</sub> O and HCl	HCN, acetylene, methane and aromatic compounds	Many different organic compounds
Waste III	e.g., SO <sub>2</sub> , CO <sub>2</sub> , NO, N <sub>2</sub> O and HCl	e.g., SO <sub>2</sub> , CO <sub>2</sub> , NO, N <sub>2</sub> O and HCl	Many different organic compounds
Waste IV	No combustion experiments were carried due to preliminary GC/MS analysis, only normal combustion products will be expected from a waste IV fire (CO, CO <sub>2</sub> , water and soot)		

Table 2  
Organic combustion products

Waste type	Organic combustion products
Waste I	Phenylacetylene; styrene; xylenes; benzonitrile; benzofurane; inden; benzylcyanide; naphthalene
Waste II	Chlorobenzene; phenylacetylene; styrene; xylenes; benzonitrile; benzofurane; benzylchloride; inden; tolylcyanide; benzylcyanide; naphthalene; biphenyle; biphenylen; naphthonitrile (isomer I + II); dibenzofurane; flourene; phenanthrene
Waste III	Phenylacetylene; styrene; inden; naphthalene; benzothiophene; biphenyle; biphenylen; dibenzofurane; dibenzothiophene; phenanthrene

the fire plume. Table 2 contains the identified organic combustion products for waste I, II and III. Tables 3–5 present the source strength for each component of waste I, II and III, respectively.

### 6.3. Discussion of uncertainties in determination of source characteristics

Uncertainties with influence on the estimated source characteristics are related to:

- collection of samples
- uncertainties in assessment of fire cases
- uncertainties in experimental work.

In total, seven samples were taken from the chemical waste. For the three waste types I, II and III, laboratory experiments showed that the composition of the two samples did not differ significantly from each other, but variations in the total bulk of chemical waste in each category have not been investigated.

A fire course can develop in different ways. In this study, the extent and course of a chemical fire has been assessed on basis of the chemicals involved and the technical configuration of the site but it is difficult in detail to predict the size of the pool, the impact from damaged drums, etc. To take this uncertainty into account two fire cases have been evaluated for each waste category: an initiating fire and a fully developed fire.

Table 3  
Source strength for each component of a waste I fire

Conditions	Initiating fire (kg/s)		Fully developed fire (kg/s)	
	B	C	A	B
Combustion rates (total)	0.2		11	
CO	0.033	0.0005	0.10	1.81
HCN	0.0005	0.0002	0.02	0.03
NO	0.0013	0.0014	0.15	0.07
N <sub>2</sub> O	0.0009	—	0.09	0.05
HCl	0.0007	0.0007	0.51	0.04
Organic compounds	0.0001	—	—	0.008



Table 4  
Source strength for each component of a waste II fire

	Initiating fire (kg/s)		Fully developed fire (kg/s)	
	B	C	A	B
Combustion rates (total)	0.02		11	
Conditions	B	C	A	B
CO	0.0049	0.0	0.06	2.7
HCN	0.0002	–	–	0.09
NO	0.0003	–	0.25	0.19
N <sub>2</sub> O	0.0002	–	0.07	0.09
HCl	0.0009	–	1.2	0.47
Organic compounds	0.0001	–	–	0.031

Table 5  
Source strength for each component of a waste III fire

	Initiating fire	Fully developed fire	Fully developed fire	
	(kg/s)	(kg/s)	(waste III + IV)	(kg/s)
Combustion rates (total)	0.003	0.3	5	
Conditions	C	C	A	B
CO	$3.0 \times 10^{-6}$	0.0003	0.01	0.03
SO <sub>2</sub>	$9.0 \times 10^{-6}$	0.0009	0.24	0.27
NO	–	–	0.03	–
N <sub>2</sub> O	–	–	0.01	–
HCl	–	–	0.05	0.03
Organic compounds	–	–	–	0.0007

Furthermore, the fire course will depend on the supply of oxygen and the combustion temperature. Simulation of fires under different conditions is time consuming and therefore three fire conditions have been selected which covers the initiating fire and the fully developed fire. The fire conditions have been selected due to recent experiences from scaling tests. The tests showed that for four different scales the production of combustion products are comparable, e.g. in the yields of HCl and dioxins. An essential uncertainty aspect is the assessment of the composition of fire plumes from realistic fires on basis of the experimental results because other physical conditions will influence the fire course as, e.g. turbulence and change of wind direction [9].

## 7. Assessment of pool fire behaviour, plume rise and atmospheric dispersion

The impact of toxic material from the fire to the environment is dominated by the atmospheric dispersion. Concentrations in the plume follow from the amount of material released (source strength), and the plume rise is determined by the heat release and the effect of nearby buildings. Further downwind, the atmospheric turbulence governs the concentration patterns. So assessment of dispersion requires analysis of the pool fire behaviour (source strength and heat release), the site characteristics and meteorology.

### 7.1. Calculation methods for fire dimensions and combustion rates

The estimates for burning rates of the fires is mainly based on information about pool fires. According to Babrauskas [10], for most fuels burning rates (effectively burning rate *fluxes*,  $\text{kg m}^{-2} \text{s}^{-1}$ ) become independent of size beyond a certain pool diameter. Babrauskas provides a correction to apply to the infinite size burning rates  $m''_{\infty}$  (which is empirical data depending on the fuel) to obtain the burning rates for smaller pool diameters. This correction involves the product  $k\beta$  of the absorption–extinction coefficient  $k$  and the ‘mean–beam–length corrector’  $\beta$ , which are also empirical fuel properties. Rew and Hulbert [11] provide tables with  $m''_{\infty}$  and  $k\beta$  for 24 widely used chemicals. In case  $m''_{\infty}$  is unknown, Rew and Hulbert as well as the TNO Yellow Book [12], refer to Burgess and Hertzberg’s method, which simply states that 0.1% of the heat of combustion is used to evaporate the fuel.

### 7.2. Combustion properties of the chemicals involved

Table 6 presents an overview of the material properties which are needed for the estimates of combustion rates. The heat of combustion is counted from the vapour phase at boiling temperature, and the heat of evaporation includes heating up the fuel (solid or liquid) to the boiling point and melting of the solid if appropriate. Except for the waste IV mixture, the products consist of chemicals for which only scarce data is available. Therefore estimates or default values have been used on the basis of assumed similarities with known chemicals. It appears that the variation in burning rates is rather small considering the poor sources of data, and it can be considered accurate within the bounds presented in Table 6. Only the initiating fires are affected a little by the  $k\beta$  correction (i.e. they have a burning rate only little less than  $m''_{\infty}$ ).

### 7.3. Meteorological situation

The different possible fire cases lead to two quite different dispersion situations. (1) Large (pool)-fires with large releases of heat will produce rapidly rising plumes. The

Table 6  
Combustion properties of the materials

	Heat of combustion (kJ/kg)	Heat of evaporation (kJ/kg)	Burning rate $m''_{\infty}$ ( $\text{kg m}^{-2} \text{s}^{-1}$ )	$k\beta$ ( $\text{m}^{-1}$ )
Waste I	33,300	498	0.051 <sup>a</sup> –0.066 <sup>b</sup>	100 <sup>c</sup>
Waste II	32,400	544	0.051 <sup>a</sup> –0.060 <sup>b</sup>	100 <sup>c</sup>
Waste III	5520	1786	0.003 <sup>b</sup>	100 <sup>c</sup>
Waste IV	32,800	756	0.043	3.37

<sup>a</sup>From Rew and Hulbert for crude oil.

<sup>b</sup>Using Burgess and Herzberg’s method.

<sup>c</sup>Default value according to Rew and Hulbert.

Table 7  
Meteorological conditions for dispersion calculations

Case	Wind at 10 m (m/s)	Surface friction velocity (m/s)	Monin–Obukhov length $L$ (m)	Mixing depth (m)
U2	2	0.291	– 19	1000
U5	5	0.601	– 169	1000
N2	2	0.228	– 10,000	500
N5	5	0.570	– 10,000	500
S2	2	0.093	9.5	34.4

highest concentrations on the ground under elevated plumes will occur during unstable atmospheric conditions. (2) Small fires with low combustion efficiencies (so with relatively large releases of toxic products) will produce plumes that will stay near the ground. The highest concentrations for ground-level plumes occur during low-wind, stable conditions.

Therefore, the following conditions have been selected for the dispersion calculations: (1) U2, an unstable case with low wind speed (2 m/s) for the study of large fires. (2) U5, an unstable case with medium wind speed (5 m/s, this will reduce plume rise to some extent) for the study of large fires. (3) N2, a neutral case with low wind speed for all fire sizes. (4) N5, a neutral case with medium wind speed for all fire sizes. (5) S2, a stable case with low wind speed for small size fires.

The unstable cases will correspond to bright days around noon in the period May–July. The stable condition will correspond to nights and mornings with clear sky and surface temperatures between 0 and 10°C. Aerodynamic properties of the site have been estimated using a variety of methods and recommendations [13–15]. The parameters for the meteorological conditions selected above have been constructed on the bases of the methods of Høltslag [16], with ‘typical’ values for the daytime mixing heights. It should be noted that these conditions are not based on considerations of frequency of occurrence rather than that they represent ‘worst’ or at least ‘serious’ case conditions. The wind speeds are according to normal Danish practice for consequence assessment studies. The key parameters for the five meteorological conditions are presented in Table 7.

## 7.4. Plume rise

### 7.4.1. Calculation methods

There is relatively little information available on the rise of fire plumes. Zonati et al. [17] compared two ad hoc models with experimental data obtained in a wind tunnel. One of these models is Moore’s formula as used by the UK Health and Safety Executive [18]. The other model is an adoption of Brigg’s plume rise model by Mills. Zonati et al. conclude that both models behave equally well compared to the experiments. Risø developed the GREAT model for jet-type of releases [19]. It is an integral type model. It appears that the plume rise predicted using GREAT is about 20% lower than that

predicted by Mills' model. In order to keep on the conservative side, GReAT-results are used as input to the dispersion calculations for the large fires.

#### 7.4.2. Building effects and lift-off

Hall et al. [20] studied the behaviour of fire plumes released from buildings. For the present case, where most fire plumes will emerge from the immediate vicinity of a pilot laboratory building, their study concerning lift-off from building wakes is relevant. Based on wind tunnel studies they conclude that lift-off can not easily be predicted and that it depends on the building shape and the releases mode. Furthermore, they observe a gradual rather than a discrete change from 'no lift-off' to 'lift-off'. If lift-off is defined as plume rise causing a reduction of a factor of 100 at ground level compared to a plume without plume rise, then a conservative estimate of lift-off can be derived from Hall's measurements by stating:

$$\frac{F}{U^3 L} > 1$$

Here  $F$  is the buoyancy flux, which can be expressed in terms of the total convective heat release of the fire:  $F = 8.9Q$  ( $Q$  expressed in MW);  $U$  is the wind speed at 10 m and  $L$  is the building height (6 m for the pilot laboratory building). For plumes which do not exceed the limit value of 1, no lift off will be assumed, and the plume height is assumed to be at a height of 0.6  $L$ , in accordance with Dutch recommendations [21].

#### 7.4.3. Results

First, the possibility of lift-off from the building wakes is assessed. Table 8 presents the wind speeds beyond which no lift-off will occur. For the calculation of the net convective heat release, it is assumed that the radiative loss is 30% for all fires. This is probably conservative for the larger fires, thus underestimating the plume rise.

Fully developed fires lift-off for wind speeds up to 7 m/s. For these fires one may question the validity of the lift-off criterion, because the fires are large compared to the building. Wind speeds of 7 m/s or more occur 13% of the time at the site. Plume rise calculations are only needed in case lift-off occurs. It appears that the maximum concentrations in case of lift-off are dominated by the mixing depth, see Table 7.

Table 8  
The lift-off criterion

Fire case	Net heat release (MW)	No lift-off beyond (m/s)
Initial waste I fire	5	< 2
Full waste I fire	254	7.2
Manhole waste II fire	0.5	< 2
Full waste II fire	240	7.1
Single drum waste III fire	0.01	< 2
Full waste III fire	1.1	< 2
Supported waste III fire	> 600	> 9.6
Single drum waste IV fire	1	< 2
Full waste IV fire	600	9.6

## 7.5. Dispersion

### 7.5.1. Calculation methods

Dispersion from the fire plume is calculated using the Gaussian plume model (see e.g. Ref. [22]), including reflection of plume material at the ground and at the mixing height.

The method to determine the dispersion parameters  $\sigma_y$  and  $\sigma_z$  is taken from the methods described in the 'Revised Yellow Book' [23]. These methods are based on the work on atmospheric turbulence by Gryning et al. [24] and the description of dispersion in the surface layer including effects of shear by Van Ulden [25]. One should consider that the Gaussian Plume model is less appropriate for unstable weather conditions because then very large vortices sweep the plume up- and downwards continuously. It is assumed that all releases for all wind directions occur from the near wake of the pilot laboratory building. Therefore an initial plume size has been assumed according to the WVl [21], which states that  $\sigma_{y0}$  equals the building width divided by 2.83, and  $\sigma_{z0}$  equals the building height divided by 2.36. The concentration is calculated for a 10-min averaging period.

### 7.5.2. Results

The effect of the pilot laboratory building is considered to be the same for all wind directions. Therefore, the calculations are limited to the concentration at ground level below plume centreline (i.e.  $y = 0$ ,  $z = 0$ ). These concentration profiles can be applied to all wind directions. The profiles are presented as  $\mu\text{g}/\text{m}^3$  per kg/s emission.

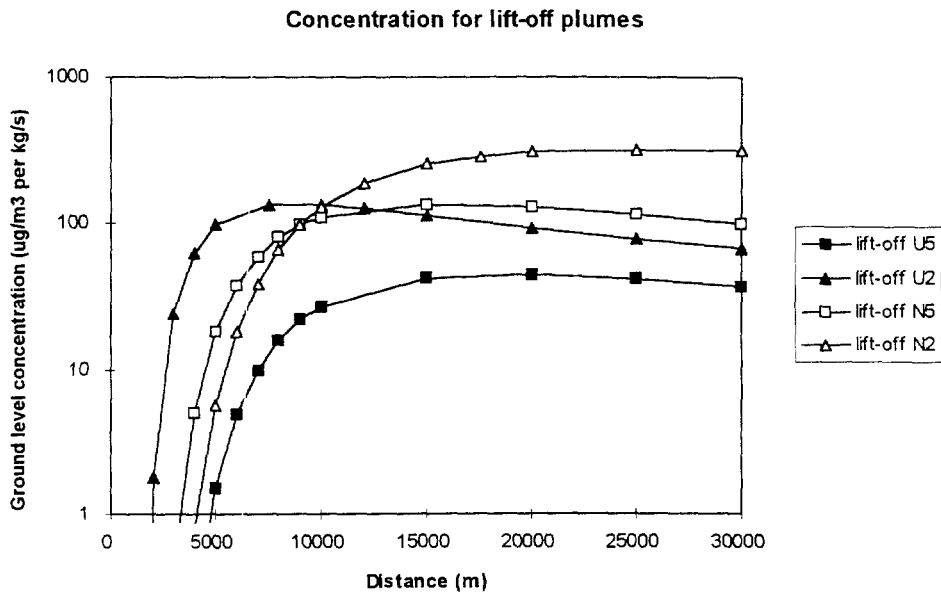


Fig. 4. Concentration as a function of down wind distance for plumes that lift off from the ground. Results are presented for unstable (closed symbols) and neutral (open symbols) conditions, and for 2 m/s (triangles) and 5 m/s (squares) wind speed.

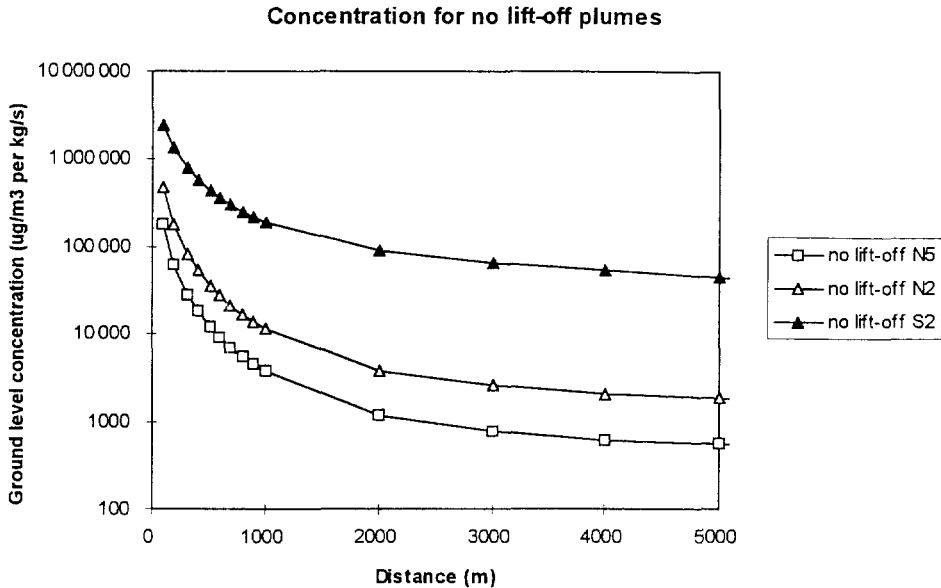


Fig. 5. Concentration as a function of distance for the plumes that do not lift off. Results are presented for neutral (open symbols) and stable (closed symbols) conditions, and for 2 m/s (triangles) and 5 m/s (squares).

Fig. 4 shows the concentration profiles for the lift-off cases. The plume rise as calculated for the fully developed waste 1 fire has been used, maximised at the mixing height. Vertical mixing is fastest for the most unstable case of U2, causing the maximum concentration to occur at a distance of about 5 km. The higher maximum concentrations for the neutral cases are caused by the lower mixing height (500 m compared to 1000 m), which reduces the volume over which the material can be distributed. The lower wind speeds (i.e. lower 'ventilation rates') lead to higher concentrations.

Fig. 5 shows the results for the no lift-off cases. Highest concentration is of course closest to the source (plume height is about half of the building height and initial dispersion in the wake of the building is accounted for). The concentration profiles are calculated from a distance of 100 m away from the fire, corresponding to the boundary of the site. The maximum concentrations occur for the stable condition due to the limited vertical mixing. The dilution of plume material is orders of magnitude less than at the position of maximum concentration in the case of the lift-off plumes:  $2.5 \text{ g/m}^3$  compared to  $300 \text{ } \mu\text{g/m}^3$  per unit emission of 1 kg/s, i.e. a factor of 8000 difference (it should be considered that the burning rates in case of lift-off are at maximum only 500–600 times more than without lift-off, and in view of the different fire characteristics the differences in emissions of toxic products will probably be less).

#### 7.6. Discussion of uncertainties in dispersion modelling

Uncertainties related to the estimated concentrations are related to:

- release of toxic material ('yield') per kg burnt fuel

- fuel burning rate
- uncertainties in lift-off and plume rise
- uncertainties in meteorological parameters
- uncertainties in the plume dispersion parameters.

The release of toxic material is discussed in Section 6, and its uncertainty will not be discussed here. The ground level concentrations are linearly proportional to the release of toxic materials. The variation in fuel burning rates for the different fuels is not very large, with exception of waste III. Therefore, the uncertainty in the burning rates is estimated as follows: waste I  $\pm 25\%$ , waste II  $\pm 25\%$ , waste III  $\pm 100\%$ , waste IV  $\pm 15\%$ . The effects of uncertainty in the burning rates are twofold: Firstly, the burning rate determines the amount of toxic material released; the concentration varies linearly with the burning rate (for fixed combustion conditions). Secondly, the burning rate determines the heat release and therefore the possible plume rise. For plumes without lift-off it will have a minor effect (buoyancy of the plume is almost irrelevant). For rising plumes, the plume rise is so strong, that a change in buoyancy will only have a minor effect (20%) on the maximum concentration and its location.

The criterion for lift-off is open for debate. In reality, there is no sharp distinction between plumes without any plume rise and plumes with full plume rise as if there was no building. One could argue the limit value should be 0.3 instead of 1. This would mean that the initial waste I fire would lift-off. For the low wind (2 m/s) cases, concentrations would then almost be as for the fully developed fire, for the 5 m/s case ('N5') the plume would level off at a height of about 200 m, leading to ground level concentrations that are a factor 10 lower than calculated without lift-off.

For the fully developed fires, not the plume rise itself, but the height of the inversion or mixing height that limits the plume rise determines the ground-level concentration. The mixing height is an uncertain parameter. An indication of the effect of the mixing height can be seen from the differences between the results for case U5 (mixing height 1000 m) and N5 (500 m) in Fig. 4.

The largest uncertainty in the application of the Gaussian plume model is related to the evolution with time and distance of the plume dispersion parameters  $\sigma_y$  and  $\sigma_z$ . Evaluations by Erbrink using parameter descriptions similar to the ones used here, showed that on a hour-by-hour comparison of measurements and model calculations there was almost no mean bias in neither ground-level concentration,  $\sigma_y$ , nor  $\sigma_z$ . However the variability is large. The 'factor of 2', i.e. the fraction of the calculations that are not more than a factor of 2 away from the measurements, is 36% for ground-level concentration.

The overall uncertainty, excluding cases affected by uncertainty in lift-off and excluding the uncertainty in the source strengths, is therefore thought to be a factor of 4 to 5.

## 8. Discussion—lessons learned

The study illustrates the applicability of laboratory experiments combined with theoretical consequence calculations, and the results of the study have afterwards been

used by the Danish EPA with respect to a toxicological assessment and recommendations concerning emergency plans.

A topic which has been discussed more than once during the study has been the dynamic behaviour of the fire starting from the ignition of the waste to the fully developed fire. Essential aspects are:

- the flammability of the waste types
- the ignition temperature and propagation of the flame for each type of waste
- how realistic are the fire cases (size of pools, plume rise, combustion limits, etc.).

A thorough description of these aspects will demand an experimental determination of physical and chemical fire characteristics for each waste type together with an assessment of ignition sources and a development of comprehensive fire scenarios which not has been possible within the resources available for the study.

An essential aspect of the study has been to consider the links between the different disciplines to ensure accordance between the input–output relations (conditions, results, etc.). Referring to Fig. 1, attention should be drawn to the interaction between ‘pool fire and dispersion’ and ‘combustion experiments’ with respect to temperature and O<sub>2</sub>-concentrations. Ideally, the conditions for the combustion experiments should be developed in an iterative process with the pool fire calculations but due to the limited project resources this has not been possible. The conditions for the combustion experiments have in this study been selected on basis of experience from other fire research projects.

The coherence of the study and the uncertainties on the results have been continuously evaluated during the project, but it has not been possible to identify the dominant source of uncertainty because for some issues the uncertainties could only be expressed qualitatively.

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