National Institute for Public Health
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Ministry of Health, Welfare and Sport

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RIVM report 2021-0120
E. Kooi | G. Laheij

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E. Kooi (author), RIVM
G. Laheij (author), RIVM

Contact:
Eelke Kooi
Environment and Safety/Centre for Safety
eelke.kooi@rivm.nl

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Synopsis

Review of the method for calculating off-site acute health risks of incidents in storage facilities for packaged hazardous substances

When companies store large quantities of packaged hazardous substances, it can lead to incidents that pose risks for residents in the vicinity. For example, if a fire breaks out, toxic fumes can be released in quantities that are life-threatening for people present in the surroundings.

Companies are therefore required to identify these risks. In the area adjacent to a company where the risks are the greatest, no “vulnerable objects”, such as houses, are allowed to be present. Outside of this area, there is another area for which the local government must decide whether the population is adequately protected or whether additional measures are needed.

The size of these two areas is calculated with a prescribed method. This method was last updated in 2009. RIVM has analysed whether the calculation method is still in line with the latest insights in the scientific literature. The conclusion is that the method can benefit from improvements on a number of points. RIVM presents recommendations for working out these points in more detail.

An important recommendation is to simplify the calculation method so that only data for which there is clarity are used and not too many details. Furthermore, the probability of a fire should be investigated more precisely because according to the literature, this is greater than is currently assumed. The method should also take better account of the extent to which hot smoke gases rise. Finally, current knowledge about the toxicity of substances must be used.

After updating the calculation method, the calculated risks close to the storage facility are likely to increase. The outer area, on the other hand, will become smaller.

Keywords: storage of hazardous substances; chemical warehouse; Seveso Directive; fire; risk assessment; consequence area; effect distance

Publiekssamenvatting

Review van de methode voor het berekenen van acute gezondheidsrisico's van incidenten in opslagen van verpakte gevaarlijke stoffen voor mensen in de omgeving

Bij bedrijven die veel verpakte gevaarlijke stoffen opslaan, kunnen incidenten gebeuren die gevaarlijk zijn voor omwonenden. Als er bijvoorbeeld brand uitbreekt, kunnen giftige rookgassen vrijkomen in hoeveelheden die voor mensen in de omgeving levensbedreigend zijn.

Bedrijven zijn daarom verplicht om deze risico's in kaart te brengen. In het gebied rond een bedrijf waar de risico's het grootst zijn, mogen geen 'kwetsbare objecten' zoals woningen staan. Daarbuiten is een gebied waarvoor overheden moeten besluiten of de bevolking voldoende is beschermd, dan wel extra maatregelen nodig zijn.

De grootte van deze twee gebieden wordt berekend met een vastgestelde methode. Deze methode is voor het laatst herzien in 2009. Het RIVM heeft onderzocht of de rekenmethode nog voldoet aan de nieuwste inzichten in de wetenschappelijke literatuur. Daaruit blijkt dat de methode op een aantal punten kan worden verbeterd. Het RIVM reikt aanbevelingen aan om deze punten verder uit te werken.

Een belangrijke aanbeveling is om de rekenmethode eenvoudiger te maken zodat er alleen gegevens worden gebruikt waar duidelijkheid over bestaat en niet te veel details. Verder moet de kans op een brand preciezer worden onderzocht omdat deze volgens de literatuur groter is dan nu wordt aangenomen. Ook moet de methode beter rekening houden met de mate waarin warme rookgassen opstijgen. Ten slotte moet de actuele kennis over de giftigheid van stoffen worden gebruikt.

Na de actualisatie van de rekenmethode zullen de berekende risico's dichtbij de opslag waarschijnlijk toenemen. Het buitenste gebied zal juist kleiner worden.

Kernwoorden: PGS15; BRZO; opslag gevaarlijke stoffen; incidenten; brand; risico; effectafstanden; aandachtsgebieden

Contents

Summary

Significant amounts of toxic substances can be released to the environment if a fire occurs in a warehouse that contains hazardous substances. Such an event therefore poses a threat to people in the surroundings of the warehouse. According to Dutch legislation, the 'off-site health risks' must be calculated if the amounts of hazardous substances that are stored in the warehouse are large. The outcomes of the risk calculation are used in the licensing process and for land-use planning.

In 1990, a method was developed to calculate the off-site health risks from toxic emissions from chemical warehouse fires. Minor changes to the calculation method were made in 1997 and 2009. The use of the method was prescribed in legislation in 2006.

In this study it was investigated whether the various elements of the calculation method are in line with current scientific insights and which elements (if any) should be updated. This investigation included a study of the literature and various model calculations.

The investigation highlighted that the assessment of warehouse fire hazards is complex. Building fires are highly dynamic and the progression of a fire depends on many variables and parameters. It depends for example on the nature and amount of the products that are stored in the warehouse, the storage configuration, the dimensions of the building, oxygen supply to the building and the effectiveness of fire suppression systems. Accounting for all these variables makes the hazard calculation highly complex and required input parameters will be open to dispute.

In the light of these difficulties and uncertainties, it is deemed impossible to calculate the risks and effects of warehouse fires with great accuracy. Calculation methods can therefore provide only rough estimates of the off-site risks and of the distances over which significant health effects can be expected.

Taking into account the above considerations, the following weaknesses in the current calculation method were identified:

- The frequency of warehouse fires was derived in 1990 and appears to be optimistic.
- The set of fire scenarios to be used in the risk calculation is large. The underlying parameters were derived from expert judgement in the late 1980s and early 1990s and lack scientific underpinning. In addition, the set of fire sizes to be used no longer reflects current fire suppression practice in cases where a fire compartment does not have an automatic fire suppression system.
- The calculation of combustion rates is sophisticated but does not take into account all the relevant parameters.
- The effect of plume lift-off due to buoyancy is not properly accounted for in the method.

- The method does not account for the release of carbon monoxide (CO), which restricts its validity.
- The probit values that are used to calculate the likelihood of fatality for toxic exposure are outdated. New probit values with a better scientific underpinning are available.
- The severity of exposure to a toxic mixture is not calculated sufficiently realistically.

Recommendations to improve the method are provided in Chapter 6 of this report.

1 Introduction

PGS15-warehouses are warehouses where significant amounts of packaged hazardous substances, including packaged hazardous waste, are stored.[1] Accidents may occur in or around these warehouses and can result in fire, explosions and the release of toxic substances to the environment. In extreme cases, persons present in the vicinity of the warehouse may experience significant negative health effects when exposed to these toxic substances.

According to Dutch legislation [1], the off-site health risks of possible industrial accidents must be in balance with the permitted land use around the associated industrial activities. For example, no residential houses or similar ‘vulnerable objects’ are allowed at locations where the individual fatality risk exceeds a value of 1×10^{-6} per year. Milder land-use restrictions apply in the zone where the individual fatality risk is lower than 1×10^{-6} per year. The requirements apply to different types of industrial activities.

A risk calculation is needed to quantify the off-site health risks of certain activities. Storage of at least 10,000 kg packaged hazardous substances in PGS15-warehouses is one of these. A guideline is available that defines how the risks must be calculated for different types of activities [2]. The level of detail in this guideline is high, leaving little room for personal interpretation.

The first version of the risk calculation method was published in 1991 [3]. It was updated in 1997 [4] and 2009 [5]. The current version of the calculation method [2] is identical to that of 2009.

According to the guideline, two types of accident scenarios should be included in the risk analysis:

i. the release of toxic combustion products and non-combusted toxic products by a fire in a warehouse;
ii. the dispersion of hazardous substances due to damage to packaging during handling in the open air.

Exposure to heat radiation from a warehouse fire is not considered in the risk analysis. Protection from heat radiation from façade fires is covered in general legislation for buildings and constructions [6].

The restrictions on land use in the zone where the individual fatality risk is below 1×10^{-6} per year are not specified in detail in the current legislation. More explicit restrictions are being formulated in the Environment and Planning Act [7], which is expected to become effective in 2022. Within a ‘maximum effects contour’, possible further measures to protect people should be considered. The Environmental Safety Handbook [8] defines how the maximum effects contour should be calculated. It uses the scenarios and assumptions of the risk calculation method [2] as a starting point.

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[1] The term ‘PGS15’ refers to the Dutch technical standard for this type of storage [10].

Using the existing calculation method, maximum effect distances for severe, possibly life-threatening, effects from a release of toxic products from a warehouse fire can be in the order of 5 km. Some stakeholders have recently claimed that such maximum effect distances are unrealistically large. This claim was the trigger to reassess the validity of the risk calculation method.

The current report comprises a review of the existing Dutch method for the calculation of the risks from (and effects of) chemical warehouse fires. Using the latest information, the relevance and validity of the scenario inputs and their underlying assumptions are re-assessed. The focus of the review is the release and dispersion of toxic combustion products from a fire. The review of dose–effect relations for toxic products is excluded from this project, as these have already been reviewed by a group of toxicologists as part of another project [9]. Specific accident data have not yet been investigated. This could be done in a follow-up to this literature review. The risk related to the dispersion of toxic substances due to damage to packaging during handling in the open air is also not discussed in this report.

Chapter 2 describes the existing Dutch risk calculation method. It presents the main components of the method, their parameters and the background to and justification of parameter choices. The outcomes of a literature survey that was undertaken to identify gaps and weaknesses in the current Dutch method are presented in Chapter 3. These weaknesses and corresponding options for improvement are further discussed in Chapter 4. Different ways to improve the dispersion modelling for buoyant releases from buildings are investigated in Chapter 5. The overall conclusions and recommendations are presented in Chapter 6.

Chemical warehouses and off-site health risks related to chemical warehouse fires

In this report, the terms ‘PGS15-warehouse’ and ‘chemical warehouse’ are used for warehouses in which at least 10,000 kg of packaged hazardous substances are stored, including packaged hazardous waste. Chemical warehouses can contain multiple fire compartments. Each fire compartment can have multiple storage sections. Chemical warehouses are subject to the Dutch technical standard for storage of packaged hazardous goods in warehouses [10]. This standard requires, for example, that the size of a storage section in a compartment should not exceed 300 m^2.

Different types of accidents may occur in chemical warehouses. This report focuses on the release of toxic products by a fire within the warehouse.

As in any other building, fires may occur in warehouses where significant amounts of packaged hazardous substances are stored. The development of such fires depends on many factors, such as the characteristics of the products that are stored in the warehouse, the layout of the storage, the availability of oxygen and the effect of fire suppression systems (when present). Toxic combustion products, such as carbon monoxide, nitrogen oxides, sulphur dioxide and hydrogen halides, can be formed in the combustion process. Non-combusted toxic products in the storage area can also be dragged into the smoke by the fire.

Toxic products may disperse to the outside environment through openings in the building that were already present prior to the fire and through openings that were created by the fire. The subsequent dispersion of these toxic products depends on volume and temperature fluxes, on the size and location of the openings, on weather and wind conditions and on the effect of the building on the wind flow around it. Depending on these factors, the smoke plume may remain close to the ground or lift off from the ground. There are various degrees of plume lift-off. Ground-level concentrations of toxic substances downwind from the building can reach life-threatening values if the smoke plume does not fully lift off from the ground. Therefore, fires in warehouses can be dangerous to people that are present in the vicinity of the warehouse.

Dutch legislation prescribes that the health risks of such fires must be quantified if the stored quantities of hazardous materials exceed certain thresholds. The outcomes of that risk assessment are used for licensing and land-use planning purposes.

2 Description of the current method

2.1 Introduction

The risk calculation method to be used for PGS15-warehouses (chemical warehouses) is specified in Chapter 8 of the Dutch guideline for off-site risk calculation [2]. The risk calculation method for chemical warehouses was initially developed in 1990 [3], [11] and was updated in 1997 [4] and in 2009 [5]. No changes have been made since 2009. The 2009 version of the Dutch guideline has been translated into English [5]. This version is referred to as 'the current version'. Chapter 8 involves the calculation method for PGS15-warehouses.

In this chapter, the various elements of the risk calculation method and their parameters are described in separate subsections. Each subsection starts with a description of the method component. Then the background to and justification of the method component are described.

According to the current version of the method, two scenarios need to be considered:

1. The release of toxic products by a fire within a warehouse. This scenario needs to be considered for fire compartments that contain combustible hazardous substances or other goods that raise the risk of fire.[2] The toxic products to be considered are toxic combustion products and non-combusted toxic products.
2. The release of highly toxic substances caused by damage to packaging during handling in the open air. This scenario needs to be considered for the loading and unloading of ADR class 6.1 packing group I materials.

Heat radiation from the building is not addressed in the off-site individual fatality risk calculation. It is assumed that building fires develop slow enough to provide time for people outside the building to escape. Separation distances can be used to prevent fires progressing from one building to another. This is covered in general legislation for buildings and constructions [6].

This report only involves a review of scenario 1. There appears to be little debate about scenario 2 and its validity. This could mean that its validity is good enough or that the contribution of this scenario to the overall calculated risk is insignificant.

The risk calculation for scenario 1 involves the following steps:

1. Determine the overall frequency of a warehouse fire.
2. Identify the fire scenarios to be used in the risk assessment, each scenario being a combination of a fire size, a ventilation rate and a duration.

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[2] In this context, combustible hazardous substances are hazardous substances, hazardous wastes or combustible pesticides that will continue to burn after the source of ignition has been removed. This definition is broader than that of flammable substances. The other goods that can raise the risk of a fire include large amounts of packaging material.

3. Determine the average molar composition of the stored products and the amount of oxygen required for combustion.
4. Determine the combustion rate for each fire scenario.
5. Determine the source term for the different toxic combustion products and non-combusted toxic products per fire scenario.
6. Calculate the outdoor dispersion of these toxic products and the resulting toxic dose for persons at different locations downwind of the warehouse.[3]
7. Calculate the likelihood of fatality associated with the calculated toxic dose.
8. Calculate the size of the risk and effect contours.

2.2 Warehouse fire frequency

The warehouse fire frequency is defined per fire compartment and depends on the type of substances that are stored in the compartment. The default frequency is 8.8×10^{-4} per year per fire compartment. For storage of substances under protection level 3 (see Section 2.3), the frequency is 1.8×10^{-4} per year. No risk calculations are required for storage under protection level 4.

2.2.1 Background and justification

The standard frequency for a chemical warehouse fire, 8.8×10^{-4} per year, was first provided in the first version of the method (1991). It was derived from fires in pesticide storages that had occurred in the Netherlands [11]. Incidents in the TNO FACTS database that occurred between 1975 and 1987 and involved pesticides were investigated for relevance. Four pesticide warehouse fires were selected. The total number of pesticide warehouses in the Netherlands was estimated to be around 350. This resulted in the standard frequency ($4/(13\times350)= 8.8\times10^{-4}$).

In 2001, an attempt was made to derive fire frequencies that distinguish between warehouses of different sizes. This attempt was unsuccessful. In 2006, an attempt was made to update the standard frequency, which industry representatives had argued was too high. A counter-argument was that, according to the existing assessment method, most fires would be of limited size: 20 m^2 or 50 m^2 and that the frequency of larger fires was therefore substantially lower than 8.8×10^{-4} per year. Following an analysis of different datasets, the conclusion was that the reliability of the data was insufficient to update the overall warehouse fire frequency (both small and large). Around the same time, it was decided that the standard fire frequency applies per fire compartment, not per storage or per building [5].

2.3 Fire scenarios

Depending on circumstances such as the cause of the fire, substances involved in the fire, storage configuration and availability of oxygen, fires in warehouses can spread at different speeds. The risk method uses a set of fire scenarios to capture the ways in which fires can progress. Each scenario consists of a representative fire size, a ventilation rate and a duration. Relative probabilities are assigned to all scenarios. Together, these relative probabilities add up to 1. The set of

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[3] As a conservative assumption, it is assumed that impacted persons are outdoors and will not or cannot take shelter or move from their location.

scenarios to be used for the risk calculation depend on the 'protection level' of the fire compartment and, if relevant, the fire suppression system used.

2.3.1 *Protection levels and fire suppression systems*

The protection level is a classification of the fire hazard in a fire compartment and is defined in the Dutch technical standard for storage of hazardous substances in warehouses [10]. As of 2016, this technical standard distinguishes four protection levels:

- Protection level 1: rapid fire detection and extinction. To be used for fire compartments in which the most hazardous substances are stored. Requires the use of automatic or semi-automatic fire extinction systems.
- Protection level 2a: prevention of fire spread to adjacent fire compartments or buildings. Requires rapid fire detection and the availability of enough cooling water.
- Protection level 3: storage of substances that do not easily ignite. No specific requirements for rapid fire detection or availability of cooling water.
- Protection level 4: storage of substances that are not flammable or cannot sustain a fire.

Protection level 1 is the only level that requires the use of automatic or semi-automatic fire extinction systems. For the other protection levels, the aim of technical measures is not to extinguish the fire but to prevent its spreading to other compartments or buildings.

2.3.2 *Scenarios to be used and corresponding probabilities*

The scenarios to be used for the different protection levels are defined in detail in the calculation method (chapter 8 of [5]). For protection level 1, the scenarios to be used further depend on the type of fire suppression system in use. In this subsection, the methodology is illustrated for protection level 1 and two distinct two automatic fire suppression systems:

- automatic hi-ex foam system using outside air (Table 1);
- automatic hi-ex foam system using inside air (Table 2).

For both fire suppression systems, five different fire sizes must be used in the risk calculation: 20 m^2, 50 m^2, 100 m^2, 300 m^2 and 900 m^2.

- For 'hi-ex outside air', only one ventilation rate and one fire duration is considered for each fire size.
- For 'hi-ex inside air', a distinction is made for doors in the warehouse being either closed or open. For most scenario's, two ventilation rates and two fire durations must be considered (see Table 2). The largest fire size (900 m^2) is assumed to occur only if doors are open. P_{open} and P_{closed} represent the relative probabilities that doors are open or closed during the fire.

Table 1 Scenarios to be used for automatic hi-ex outside air fire suppression

Effectiveness	Fire size (m^2)	Ventilation rate (/hr)	Duration (min.)	Relative probability
Fully eff.	20	∞	10	0.89
Partially eff.	50	∞	10	0.09
Partially eff.	100	∞	10	0.01
Partially eff.	300	∞	30	0.005
Not eff.	900	∞	30	0.005

Table 2 Scenarios to be used for automatic hi-ex inside air fire suppression

Effectiveness	Fire size (m^2)	Ventilation rate (/hr)	Duration (min.)	Relative probability
Fully eff.	20	4	10	$0.89 \times P_{closed}$
Partially eff.	20	∞	30	$0.89 \times P_{open}$
Partially eff.	50	4	10	$0.09 \times P_{closed}$
Partially eff.	50	∞	30	$0.09 \times P_{open}$
Partially eff.	100	4	10	$0.01 \times P_{closed}$
Partially eff.	100	∞	30	$0.01 \times P_{open}$
Partially eff.	300	4	30	$0.005 \times P_{closed}$
Partially eff.	300	∞	30	$0.005 \times P_{open}$
Not eff.	900	∞	30	0.005

In Table 1 and Table 2, the likelihood of a scenario decreases with fire size. This is not the case for all types of fire suppression. The likelihood of a specific fire size is derived from the time required to detect the fire, the time required to start fire suppression and the likelihood of successful suppression given these detection and response times. These parameters were estimated separately for each type of fire suppression system. More details are provided in Section 2.3.3.

The scenario duration is either the time required to extinguish the fire (if applicable) or the time until significant plume lift-off starts to occur. A cap of 1800 s is applied.

- The time required to extinguish the fire depends on both the fire size and the ventilation rate (i.e. the availability of oxygen). Normally, oxygen supply should be restricted by closing doors. The possibilities of doors being closed or open are both considered. For hi-ex outside air (Table 1), the oxygen supply to the fire is always unrestricted, and no distinction is made between different ventilation rates.
- Significant plume lift-off is expected to occur once the building structure starts to lose its integrity. This is assumed to occur after 1800 s.

Notes:

- For most fire suppression systems under protection level 1, both a ventilation rate of 4 building volumes per hour and an unrestricted ventilation rate (∞) should be assumed. If the doors are closed for the duration of the fire, the ventilation rate is 4. If the doors do not shut during the fire, the ventilation rate is unrestricted. The probability of the doors not shutting depends on the type of door:

  - Automatic self-closing fire doors: $P_{closed} = 0.98$, $P_{open} = 0.02$.
  - Manually operated doors: $P_{closed} = 0.9$, $P_{open} = 0.1$.
- Some fire suppression systems, e.g. automatic hi-ex foam systems using outside air, have smoke and heat exhaust ventilation equipment (smoke vents). For these systems, the air flow into the warehouses is unrestricted. An unrestricted supply of oxygen is also assumed for warehouses that do not have an automatic fire suppression system.
- When the ventilation rate is 4 volumes per hour, the largest fire area is 300 m^2. Larger fires can be effectively sustained (assuming a fixed combustion rate per unit area) only if enough oxygen is available, i.e. if the ventilation rate is greater than 4 volumes per hour.
- The maximum fire area is normally equal to the size of the fire compartment. A smaller maximum can be used if a part of the fire compartment is exclusively reserved for the storage of products that are non-combustible or otherwise cannot contribute to the fire. The total floor size should be used if the storage facility does not meet the requirements of the PGS15 technical standard.
- If no spray cans are stored, it is assumed that significant plume lift-off occurs if the fire size exceeds 900 m^2. Fire sizes larger than 900 m^2 are then not considered.
- Different fire sizes apply if spray cans are stored and rocketing of spray cans to other parts of the fire compartment is not adequately prevented. Rocketing of spray cans can result in much faster fire development. Only two fire scenarios are then considered: the minimum fire size (20 m^2) and the full size of storage area. The relative probability for the latter size is 1 minus the probability of fire size 20 m^2.

2.3.3 *Background and justification*

The first risk calculation method [3] was the result of a prior research project [11]. The current method [5] uses the general approach that was outlined in the first version of the risk calculation method. This general approach consisted of the following steps:

1. Identify which type of fire suppression system applies to the fire compartment.
2. Identify the relevant fire sizes to be considered and the likelihood of each fire size.
3. Identify per fire size the ventilation rates and the fire durations to be used, and their relative probabilities.

2.3.3.1 Types of fire suppression systems

In the first version of the method, six types of fire repression system were distinguished. All these types belonged to protection level 1 (see Section 2.3.1).

- automatic sprinkler system;
- automatic deluge system;
- automatic gas extinguishing system;
- automatic hi-ex foam system;
- in-company fire brigade – manual deluge system;
- in-company fire brigade – interior fire attack.

Scenarios for protection levels 2 and 3 were added in 1997. Fire suppression using an automatic or semi-automatic monitoring system was added in 2009.

In 2016, the Dutch technical standard for storage of hazardous substances in warehouses [10] was updated. This update also comprised a new hierarchy of protection levels:

- Protection level 1: rapid fire detection and suppression. To be used for fire compartments in which the most hazardous substances are stored. Requires the use of automatic or semi-automatic fire suppression systems.
- Protection level 2a: prevention of fire spread to adjacent fire compartments or buildings. Requires rapid fire detection and the availability of enough cooling water.
- Protection level 3: storage of substances that do not ignite easily. No specific requirements for rapid fire detection or availability of cooling water.
- Protection level 4: storage of substances that are not flammable or cannot sustain a fire.

Automatic or semi-automatic suppression systems are required only for protection level 1. For the other protection levels, the focus is not on extinguishing the fire in the compartment but on preventing it from spreading to other compartments or buildings.

2.3.3.2 Fire size

The approach from the earliest version of the risk calculation method onwards was to link estimated response times and effectiveness of fire suppression systems (or approach) to fire sizes and durations. For example, a building provided with an automatic fire suppression system would have a relatively high probability of a small fire and a relatively small probability of a large fire. In contrast, indoor fire attack by a local fire brigade would have a relatively high probability of a large fire and a relatively low probability of a small fire.

The assumptions for different types of suppression systems are illustrated in the next subsections. In general, the maximum fire size was 20 m^2, 50 m^2 or 100 m^2 if fire suppression was (partly) successful. If fire suppression was not successful, the fire could grow to a larger size. In the consequence and risk calculation, a cap of 300 m^2 was then used for the maximum fire size. The maximum fire size to be considered is further discussed in Section 2.3.3.4.

The relative probabilities of different fire sizes were first derived for fire suppression by an automatic sprinkler system. The relative probabilities for other fire suppression systems were then derived from those for the automatic sprinkler system, using qualitative comparisons.

2.3.3.2.1 Fire suppression by automatic sprinkler systems, automatic deluge and hi-ex foam systems, and automatic gas extinguishing systems

A questionnaire was used to assess the likelihood of different fire sizes for warehouses using automatic sprinkler systems [11]. The likelihood that fire suppression would be unsuccessful was estimated to be 1%. The remaining 99% were distributed between fire sizes of 20 m^2, 50 m^2 and

100 m^2. As the response time of an automatic system is short, the likelihood of a relatively small fire (20 m^2) is relatively high (45% from 99%).

Table 3 Initial fire size probability distribution for automatic sprinkler systems

Fire size	**Likelihood**
20 m^2	0.45
50 m^2	0.44
100 m^2	0.10
Maximum size (300 m^2)	0.01

On account of a lack of further data, the values of Table 3 were also assumed to be applicable to automatic deluge systems and for automatic hi-ex foam installations. In 1997, specific values were derived for deluge and hi-ex foam systems, using qualitative comparisons of the response times and the expected effectiveness of these systems, compared with those for automatic sprinkler systems [4]. These values are listed in Table 4.[4]

Table 4 Fire size probability distributions for automatic deluge and hi-ex foam systems

Fire suppression system	**20 m^2**	**50 m^2**	**100 m^2**	**≥ 300 m^2**
Automatic deluge system	0.63	0.26	0.10	0.01
Automatic hi-ex foam system	0.89	0.09	0.01	0.01

Automatic gas extinguishing systems were supposed to either stop the fire within 5 minutes or not be effective at all. The likelihood of effective suppression was assumed to be 99% and the corresponding fire size 20 m^2 [11].

Table 5 Fire size probability distribution for automatic gas extinguishing systems

Fire size	**Likelihood**
20 m^2	0.99
Maximum size (300 m^2)	0.01

2.3.3.2.2 Suppression by in-company fire unit

For manual activation or suppression by an in-company fire unit, three distinct types of suppression were identified in [11]. For each type, the likelihood of successful/unsuccessful suppression was estimated. In addition, the response time of the system was estimated and compared with the response time of an automatic sprinkler system in a qualitative manner. Higher response times led to a lower relative probability of a 20 m^2 fire and higher relative probabilities of 50 m^2 and 100 m^2 fires.

- Manual activation of a deluge system. The likelihood of successfully manually activating a deluge system was estimated to be 90%. This value was a default for human success/failure for actions under considerable time stress. As manual activation requires more time than automatic activation, the likelihood of 50 m^2 and 100 m^2 fires is larger and that for 20 m^2 is smaller (when compared with automatic activation).
- Manual activation of a dry sprinkler system. This requires more complex actions under considerable time stress. The likelihood of

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[4] In 1997, the maximum possible size of a fire was also increased; see Section 2.3.3.4.

success was therefore reduced to 50%. As the response time is larger than for automatic systems and wet systems, the smallest fire scenario (20 m^2) was not deemed realistic.
- Indoor fire attack. For an indoor fire attack, it was assumed that there was a 50% likelihood of success, accounting for the complex tasks and the considerable time stress. When successful, the maximum fire size would be 50 m^2 or 100 m^2 (equal distribution). When unsuccessful, the fire would grow to the maximum size (≥ 300 m^2).

Table 6 Initial fire size probability distribution for manual activation or suppression (in-company)

Type of suppression	**20 m^2**	**50 m^2**	**100 m^2**	**300 m^2**
Manual activation of a wet deluge system	35%	45%	10%	10%
Manual activation of a dry deluge system		40%	10%	50%
Indoor fire attack		25%	25%	50%

In the 1997 update of the method [4], the relative fire size probabilities for manual activation of a dry deluge system and for indoor fire attack by an in-company fire unit were slightly modified (see Table 7). The modifications were due to a reassessment of the complexity of these operations. In addition, the maximum fire size criteria were modified in 1997; see Section 2.3.3.4.

Table 7 Updated fire size probability distribution for manual activation or suppression (in-company)

Type of suppression	**20 m^2**	**50 m^2**	**100 m^2**	**≥ 300 m^2**
Manual activation of a dry deluge system		20%	30%	50%
Indoor fire attack		20%	30%	50%

The Dutch technical standard for the storage of hazardous substances in warehouses was updated in 2016 [10]. In that update, indoor fire attack was no longer considered as an option. To rapidly extinguish a fire, the fire compartment should be equipped with an automatic or semi-automatic fire extinction system. In the absence of such a system, the focus of mitigation actions will be to prevent fire spread to adjacent compartments or buildings.

2.3.3.2.3 Protection levels 2, 3 and 4

In 1997, new sets of scenarios were derived for protection levels 2 and 3, that is, for fire suppression by the local fire brigade with limited preparation. For protection level 2, the distribution of likelihoods depends on the presence (or not) of flammable liquids (ADR class 3 products) in plastic containers.

Table 8 Fire size probability distribution for manual activation or suppression

Type of suppression	20 m²	50 m²	100 m²	≥ 300 m²
Response time <6 minutes, ADR 3 in plastic containers				100%
Response time <6 minutes, no ADR 3 in plastic containers		20%	30%	50%
Response time <15 minutes, ADR 3 in plastic containers				100%
Response time <15 minutes, no ADR 3 in plastic containers				100%
Fire attack by local fire brigade				100%

The hierarchy of protection levels was modified in the 2016 version of the Dutch standard for the storage of hazardous substances in warehouses [10]. Protection level 2 was replaced by protection level 2a and protection level 4 was added as an additional protection level. Automatic or semi-automatic fire suppression systems are required only for protection level 1.

For protection levels 2a, 3 and 4, the focus is not on extinguishing the fire but on preventing the fire from spreading to other compartments or buildings. New guidance was provided for the new protection levels:

- For protection level 2a, only the largest fire size must be considered. The relative probability of that fire size is 1.[5]
- For protection level 4, the fire hazard is limited and no risk calculation needs to be carried out.

The scenarios for protection level 3 were not updated.

2.3.3.3 Ventilation rate

The ventilation rate is relevant for the combustion rate (Section 2.5). If there is a lack of air (oxygen), the combustion rate will be oxygen-restricted. The resulting combustion rate can be derived from the amount of oxygen available for combustion.

The 1991 version of the calculation method assumed a default ventilation rate of 4 building volumes per hour. For automatic gas extinguishing systems, zero ventilation was assumed, unless doors in the warehouse would fail to close. In the latter case, the ventilation rate was assumed to be 4 building volumes per hour, also taking into account a possible ‘suction effect’ of a fire. For hi-ex foam systems with outside air and for indoor attack, the ventilation rate (oxygen supply) was assumed to be infinite.

In 1997, it was decided to also consider the option that doors would remain open for automatic sprinkler and deluge systems and hi-ex foam installations with inside air. Standard likelihoods for door closure were proposed in [4] (Table 9). If doors remain open, oxygen supply to the fire is assumed to be unlimited (infinite ventilation rate). The same now also applied to automatic gas extinguishing systems.

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[5] Since 2009, the largest fire size that must be considered is equal to 900 m².

Table 9 Likelihood of door closing

Type of door closing	Likelihood of success
Manual closing of doors in case of fire	90%
Automatic closing of doors in case of fire	98%

2.3.3.4 Maximum fire size

In the first version of the risk calculation method, the maximum fire size to be considered was 300 m^2. Limited justification was provided for this maximum fire size. It was said to be in line with the expectation that plume rise would start to occur after 20 or 30 minutes, depending on the construction of the warehouse. An additional argument was that larger fire sizes would not necessarily result in higher source terms, because combustion for sizes beyond 300 m^2 would normally be oxygen-restricted. The combustion rate for a fire of 300 m^2 with infinite oxygen supply was therefore considered to be a reasonable conservative maximum.

In the 1997 update of the calculation method [4], the cap of 300 m^2 was removed, because it was believed that larger fire sizes could also be relevant. Depending on the total size of the fire compartment, additional fire sizes of 900 m^2, 1600 m^2 and 2500 m^2 now also had to be considered.[6] The maximum size of 2500 m^2 referred to the largest fire compartment size allowed at the time.[7] It was believed at the time that such large fires could also continue for at least 30 minutes without significant structural collapse of the building and/or significant plume lift-off. However, no explicit references were made to the time required to reach such larger fire sizes, the conditions when buildings would collapse or the buoyancy of the associated releases.

New probability distributions were derived for the fire sizes beyond 300 m^2. For (semi-) automatic sprinkler, deluge and hi-ex foam systems, the distribution for fire sizes of 300 m^2 and larger was copied from Table 4, i.e. 0.50 : 0.40 : 0.09 : 0.01, multiplied by the total probability of a (large size) fire of 300 m^2 or more (P_{ls}). This probability distribution was somewhat arbitrary as it initially applied to the size distribution of small fires suppressed by an automatic sprinkler system. For indoor attack, the probability distribution was more or less inversely proportional to the fire size, if the response time was less than 6 minutes. For longer response times, somewhat more conservative probability distributions were used, without detailed explanation of their origin.

Table 10 Fire size probability distribution from 300 m^2 onwards for the use of (semi) automatic fire suppression systems ([4])

300 m^2	900 m^2	1600 m^2	2500 m^2
P_{ls}×50%	P_{ls}×40%	P_{ls}×9%	P_{ls}×1%

In the 2009 update [5], the maximum fire size was reassessed. If liquid spreading to adjacent storage sections was prevented by technical measures (e.g. separate containment provisions per section for liquid

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[6] The actual size of the storage area is the true maximum. This can be smaller than 2500 m^2. All sizes smaller than the storage size must be considered, as well as the storage size itself.

[7] Lower maximum storage sizes applied to automatic gas extinction systems (600 m^2), automatic hi-ex systems (1500 m^2), indoor attack by in-company fire brigade (1500 m^2) and use of dry deluge system by local fire brigade (300 m^2).

spills), the maximum fire size deemed relevant for the risk calculation could be restricted to 900 m^2. This modification was justified by two arguments. First, separation distances between different storage areas[8] should limit the propagation of the fire. It was assumed that within the first 1800 s[9] the fire could not reach sizes of 1500 or 2500 m^2. Second, it was presumed that fires not only grow during the early stages, but also move. The active combustion zone would then be smaller than the area involved in the fire.

The maximum fire size of 900 m^2 does not apply if spray cans are stored without measures to prevent the rocketing of these cans to neighbouring sections. If no adequate measures have been taken to prevent rocketing, the maximum fire size is equal to the storage area size (see notes in Section 2.3.2).

2.3.3.5 Scenario duration

In the first version of the risk calculation method, the scenarios with a fire size of 100 m^2 or less would represent situations in which the fire could be extinguished. The size of 300 m^2 was a maximum size for fires that could not be extinguished.

- For fire sizes up to 100 m^2, the scenario duration was equal to the time required to extinguish the fire, with a maximum of 30 minutes.[10] This duration would be 5 minutes for automatic gas extinguishing systems, 15 minutes for automatic hi-ex foam systems and 30 minutes for all other fire repression systems.
- For the fire size of 300 m^2, the scenario duration was equal to the time required for full development of the fire, with a maximum of 30 minutes (see footnote 10). Full development would mean either structural collapse of the building or significant plume rise. For buildings with little fire resistance, the time until structural collapse occurred was estimated to be 20 minutes. The cap of 30 minutes applied to buildings that were designed to withstand a fire for at least 30 minutes.

In 1997, the maximum fire size was increased to the maximum size of a storage compartment (see Section 2.3.3.4), which could be as much as 2500 m^2. The duration of these larger fire sizes was either 20 or 30 minutes, depending on the fire-resisting capacity of the compartment.

In 2009, in response to new standards for chemical warehouses[11], it was no longer considered possible for buildings to collapse within 20 minutes. For the corresponding scenarios, the duration was therefore changed to 30 minutes. This was the same maximum scenario duration as for all other activities for which off-site risk needs to be calculated [2].

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[8] According to the Dutch technical guidance for the storage of packaged hazardous materials [10], an individual storage section may not be larger than 300 m^2. Different storage sections should be separated from each other by a separation distance of at least 3.5 m or a structure with a fire resistance of at least 30 minutes.

[9] After 1800 s, plume rise is assumed to occur.

[10] 30 minutes is a commonly used maximum for the release duration in various Dutch risk calculation methods.

[11] In the new standards, all chemical warehouses should have a fire resistance of at least 60 minutes.

2.4 Combustion rate

2.4.1 *Calculation of the combustion rate*

The combustion rate is the amount of material that burns per unit of time (in kg/s). It is assumed that the combustion rate is uniform across the fire. It depends on the mass fraction of flammable liquids in the storage, the fire size and the availability of oxygen.

The combustion rate is calculated as follows:

- First, the 'fuel-restricted' combustion rate $\dot{m}_{FR}$ is calculated. This is the combustion rate in excess of oxygen.
    - For flammable liquids (ADR class 3) the assumed combustion rate per unit area is 0.1 kg/m^2·s.
    - For all other combustible materials, the assumed combustion rate per unit area is 0.025 kg/m^2·s.
    - The average combustion rate per unit area is the linear combination of the two and depends on the fraction of flammable liquids in the storage area.
    - The total combustion rate in excess of oxygen is the product of the average combustion rate per unit area and the fire size (see equation 1).

    $$\dot{m}_{FR} = (0.025 + 0.075 \cdot f_{\mathrm{ADR3}}) \cdot A \qquad (1)$$

    where:
    $\dot{m}_{FR}$: the (fuel-restricted) combustion rate in excess of oxygen, in kg/s
    f_{ADR3}: the mass fraction of ADR class 3 flammable liquids,
    A: the fire size, in m^2.
- Then the oxygen-restricted combustion rate $\dot{m}_{OR}$ is calculated.
    - The mass of oxygen that is required for combustion (kg oxygen/kg fuel) is determined by assuming complete combustion. Molecular bonded oxygen will be consumed during combustion. All other oxygen required for combustion is withdrawn from air.
    - The mass of oxygen available in air (kg) is the sum of the initial oxygen mass in the warehouse and the mass of oxygen that is added by ventilation. The summed mass of oxygen is divided by the fire duration to give a value in kg/s.
    - The oxygen-restricted combustion rate (kg/s) is the combustion rate for which the oxygen demand (kg/s) balances the oxygen supply (kg/s).
- The effective combustion rate is the lesser of the combustion rate in excess of oxygen ($\dot{m}_{FR}$) and the oxygen-restricted combustion rate ($\dot{m}_{OR}$).

The effect of the storage configuration, e.g. the height of racks, on the combustion rate is not normally considered. An alternative combustion rate may be used if it can be justified with specific data.

2.4.2 *Background and justification*

2.4.2.1 Fuel-restricted combustion rate

In the first version of the risk calculation method [11], the fuel-restricted combustion rate per unit area was assumed to be 0.025

$kg/m^2 \cdot s$. This average value was first proposed in [13], using the information below:

- Evaporation rate per unit area for plastics: typically between 0.005 and 0.025 kg/m^2 s.
- Evaporation rate per unit area for liquids: typically around 0.1 kg/m^2 s.
- Evaporation rate per unit area for pesticides: typically around 0.02 kg/m^2 s.

In 2009, it was decided that the maximum fuel-restricted combustion rate should be increased if ADR class 3 flammable liquids were stored in the fire compartment [5]. For ADR class 3 flammable liquids, a combustion rate per unit area of 0.1 $kg/m^2 \cdot s$ was proposed. That value was previously reported in [13]. The average combustion rate for the fire compartment should be derived from the mass fractions of flammable liquids and other materials, where the former would have an average combustion rate of 0.1 $kg/m^2 \cdot s$ and the latter a combustion rate of 0.025 $kg/m^2 \cdot s$.

The fuel-restricted combustion rate depends only on the fraction of flammable liquids in the fire compartment. (The possible relevance of the storage height, the presence of flammable solids (ADR class 4) and the presence of oxidising substances (ADR class 5) has not yet been investigated.)

2.4.2.1.1 Automated Storage and Retrieval Systems (ASRS)

Traditionally, pallets, boxes, drums, sacks, etc. were placed in the storage using forklift trucks. The storage height was then limited to the maximum height that could be reached with these trucks. In the last two decades, ASRS have been introduced. In ASRS, goods are placed in parallel racks or carousels by automated lifts, so that the storage height can be substantially greater than in traditional warehouses. The possible impact of increased storage height on the fuel-restricted combustion rate per unit area has not yet been investigated.

2.4.2.2 Oxygen-restricted combustion rate

In case of lack of oxygen, the combustion rate will be oxygen-restricted. The resulting combustion rate can be derived from the amount of oxygen available for combustion. The following oxygen contributions are considered (see also Section 2.3.3.3):

- The amount of oxygen that is present in the building prior to the fire. This amount is consumed at an even rate during the duration of the fire.
- The amount of oxygen that is added to the building via ventilation (doors closed) or via open doors. If doors are closed, the ventilation rate is 4 building volumes per hour (4/3600 volumes per second). If doors are open, the oxygen supply is assumed to be infinite.

Further notes:

- Oxygen supply due to structural collapse of the building is not considered. Instead it is assumed that the plume will lift off once the building has collapsed. No risk assessment is required for that stage of a fire; see Section 3.2.5.

- Automatic gas extinguishing systems can be effective only if the building is fully closed. The scenario for successful suppression (fire size 20 m^2) is therefore linked to successful closing of doors. The standard mechanical ventilation rate of 4 building volumes per hour is still applied in order to derive a source term. Ineffective fire suppression is divided 50/50 between ineffective suppression in a closed building (ventilation 4 per hour) and in a partly open building (infinite ventilation).

2.5 Source term

The source term is the emission rate of toxic combustion products and non-combusted toxic products released by the fire.

2.5.1 Toxic combustion products

The formation of toxic combustion products depends on the composition of the materials in the fire. The material composition may be time- and location-specific. As a starting point, the method uses the annually averaged material composition of the entire fire compartment. If the types of substances stored vary significantly during the year, it should be checked that this assumption does not result in an underestimation of risk. Differences in the material composition in different subareas of the fire compartment are not normally accounted for.[12]

Fixed conversion factors are assumed for nitrogen, chlorine, bromine, fluorine and sulphur.

- Nitrogen is assumed to produce nitrogen dioxide (NO_2) with a conversion factor of 0.1. The remainder of the nitrogen reacts to chemical compounds that are less toxic than nitrogen dioxide. These other reaction products do not have to be considered in the risk assessment.
- Sulphur is assumed to form sulphur dioxide (SO_2), also with a conversion factor of 1.
- Chlorine, bromine and fluorine are assumed to form hydrogen chloride (HCl), hydrogen bromide (HBr) and hydrogen fluoride (HF), with a conversion factor of 1. For convenience, the molar fractions of HBr and HF are combined with that of HCl in subsequent dispersion and effect calculations.
- Other toxic combustion products are normally ignored.

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[12] It can be used if detailed requirements for material composition are included in the warehouse permit.

The source terms for NO_2, SO_2 and HCl are then equal to:

$$\dot{m}_{NO_2} = 0.1 \cdot f_N \cdot \frac{46{,}01}{14{,}01} \cdot \dot{m} \tag{2}$$

$$\dot{m}_{SO_2} = 1 \cdot f_S \cdot \frac{64{,}06}{32.06} \cdot \dot{m} \tag{3}$$

$$\dot{m}_{HCl} = 1 \cdot f_{Cl} \cdot \frac{36{,}46}{35{,}45} \cdot \dot{m} \tag{4}$$

where:
$\dot{m}_p$: the source term for toxic component p, in kg/s
f_N: the mass fraction of elemental nitrogen in the fuel
f_S: the mass fraction of elemental sulphur in the fuel
f_{Cl}: the mass fraction of elemental chorine, bromine, iodine and fluorine in the fuel
$\dot{m}$: the effective combustion rate, in kg/s.

2.5.2 *Non-combusted toxic products*

A fraction of the products that are stored will be released and emitted without being combusted. This fraction is commonly referred to as the ‘survival fraction’. The survival fraction is assumed to depend on the storage height, the fire size and the type of fire suppression system used. The survival fraction for toxic liquids and powders is provided in Table 11. For toxic solids other than powders, e.g. granulates, a survival fraction of 1% should be used regardless of the storage height.

The emission of non-combusted products is considered only for toxic substances of ADR class 6.1 packaging group I and II. In addition, the quantity stored should exceed 5 or 50 tons, respectively.

Table 11 Survival fraction for toxic liquids and powders

Fire suppression system	**Fire size (m^2)**	**Storage height ≤1.80 m**	**Storage height >1.80 m**
Protection level 1: *All systems except automatic hi-ex outside air and company fire unit – indoor fire attack*	≤ 300	10%	30%
Protection level 1: *All systems except automatic hi-ex outside air and company fire unit – indoor fire attack*	> 300	1%	10%
Protection level 1: *Automatic hi-ex outside air or company fire unit – indoor fire attack*	All	1%	10%
Protection level 2	All	1%	10%
Protection level 3	All	1%	10%

For the emission rate, it is assumed that the relevant toxic products are distributed uniformly across the warehouse floor area. The emission rate is then equal to the product of the effective combustion rate (Section 2.5), the mass fraction of relevant toxic products (relative to the total mass in storage) and the survival fraction.

2.5.3 *Background and justification*

The relevant toxic combustion products for warehouses containing pesticides were initially investigated in 1991 [11]. From this survey NO_2, HCl and SO_2 were identified as being the most relevant toxic combustion products. If products contain fluorine, bromine and iodine, HF, HBr and HI can be produced in a fire. According to [11], these combustion products could be added to the source term for HCl and would not need to be studied individually.

The conversion percentage into SO_2 and HCl for sulphur- and chlorine-containing products is 100%. These conversion percentages were investigated in a literature survey in 1998 [14] and have not been reviewed or updated since.

The calculation method assumes that nitrogen in the fuel is converted into nitrogen dioxide (NO_2). The source term for nitrogen dioxide is assumed to also include emissions of other nitrogen-based combustion gases such as NO, N_2O, NH_3 and HCN. The conversion factor used for the sum of these gases was initially based on a literature study by RIVM in 1995 [15]. An average conversion of about 10% was found, with a maximum of 35% for ammonium nitrate. Due to uncertainties about the non-combusted material and other nitrogen-containing combustion products, a decision was made at that time to add a 25% safety margin to the average value of 10%. This gave a conversion percentage of 35%.

As part of the revision of the calculation method in 2009, the 35% conversion percentage for nitrogen-containing compounds was re-evaluated, with specific focus on the formation of HCN. An extensive literature study was carried out and various experts from the Netherlands and elsewhere were consulted [16]. As a result of this study, a value of 10% was adopted for the total conversion percentage from nitrogen-containing compounds to NOx and HCN. This percentage was considered to be sufficiently conservative by the national and international experts consulted.

The nitrogen-containing toxic combustion products released are treated as NO_2 in the model. Although HCN is more toxic than NO_2, the effects of a release of HCN are hardly greater because its higher toxicity is compensated for by a lower molar mass and therefore a lower source strength.

In the analyses above, it was assumed that hazardous substances are stored in dedicated fire compartments, and that these compartments contain only hazardous substances and their packaging. This assumption was in accordance with the Dutch requirements for storage of packaged hazardous substances at the time. Since 2016, both general trade goods and hazardous substances can be stored in the same fire compartment. The possible effect of this change on the type of combustion products that can be released has not yet been investigated.

2.6 Release and dispersion

Only the emission of toxic products is considered. The emission rates were discussed in Section 2.6. They depend on fire size, product composition, oxygen availability and combustion rate.

2.6.1 Indoor cooling and dilution

The current method considers only the release of toxic products in the fire; the formation of non-toxic combustion products is ignored. Indoor dilution of the toxic products is also ignored. A simple assumption is used for indoor cooling. Is it assumed that the toxic products produced in the fire will be emitted from the building at a temperature of 50 ºC.

2.6.2 Mixing in the recirculation zone and subsequent dispersion

The method further assumes that the released toxic products first mix in the recirculation zone (building wake) before dispersing further. This mixing results in the dilution and cooling of the toxic products. The model also assumes that smoke will leave the building wake as a neutrally buoyant plume.

For the risk calculations, the building shape and its orientation to the wind are simplified. The building is assumed to be square with one of its sides facing the wind (i.e. no wind angle). The height of the building and the square root of its surface area define the size of the recirculation zone.

The unified dispersion model of SAFETI-NL is used to calculate dispersion.[13] The neutrally buoyant plume that leaves the building wake is modelled with a Gaussian dispersion model. The dispersion then depends on atmospheric stability, wind speed and the assumed surface roughness of the environment.

2.6.3 Background and justification

2.6.3.1 Mass flux

Only the release of toxic products is considered in the current method. Non-toxic products, that are produced in the fire or are entrained within the building, are ignored. The motivation for this is unknown. However, as the smoke plume is assumed to be neutral and passive (see Sections 2.7.3.4 and 2.7.3.5), the effect of neglecting a part of the volume flux is limited.

2.6.3.2 Release temperature

The temperature of the released smoke was considered in annex 2 of the research report that was used to develop the first version of the risk calculation method [11]. The temperature in the seat of the fire was expected to increase to 800 ºC within 30 minutes, and to 1100 ºC after 3 hours. Above the flames, the smoke temperature would rapidly decrease. A value of 250 ºC was deemed appropriate for smoke 3 metres above the flames.

In the first version of the method [3], the smoke temperature was not further used. The emitted smoke would mix and cool in the recirculation zone and then disperse as a neutrally buoyant plume; see Sections 2.7.3.3 to 2.7.3.5.

[13] The software version to be used is specified in the guidance for risk calculation.

From 2006 onwards, following the publication of new Dutch legislation, risk calculations had to be carried out with the software programme SAFETI-NL. A specific warehouse model was included to calculate the risk of the release of toxic combustion products from chemical warehouses. As requested by RIVM, the release temperature of the toxic combustion products was set at 50 ^{0}C. The release temperature did not appear to be have a significant effect on SAFETI-NL outcomes. This insensitivity to the release temperature is related to the use of the building-wake model of SAFETI-NL. The building-wake model was developed for neutral dispersion and neglects possible gravity effects such as buoyancy (see Chapter 4).

2.6.3.3 Dilution in the recirculation zone

The fire scenarios to be considered apply to situations in which the warehouse is (largely) undamaged. After leaving the building, the released toxic products are assumed to enter the recirculation zone behind the building (building wake). The specific release location is therefore irrelevant.

Mixing in the recirculation zone had been taken into account since the first version of the risk method in 1991.

- Initially, the ‘Short Distance Immissions’ model was used to calculate this mixing. The reference for that model could not be retrieved.
- In 1997, it was decided to model the release as surface area sources, with length and width equal to the square root of the building area. This approach appears to have been a workaround for using a dedicated building-wake model.
- Since 2006, the building-wake model in SAFETI-NL has been used to calculate dispersion. The description of that model is included in the documentation that comes with the software [20].

In SAFETI-NL, it is currently not possible to used different wind angles for risk calculation. The risk calculation depends on a fixed wind angle defined by the user. The Dutch risk calculation method [5] prescribes that the building should be made square, i.e. with identical width and length, both equal to the square root of the surface area. This is a workaround to obtain average values for different building–wind orientations.

2.6.3.4 Buoyancy and plume lift-off

Buoyancy and plume lift-off were discussed in annex 2 of the research report [11] that was used to develop the first version of the risk calculation method [3]. Assessing buoyancy and plume rise was, however, not required in the resulting risk calculation method because the scenarios to be used in the risk assessment were supposed to represent situations with limited or no plume rise. To not consider plume rise at all, was a conservative simplification.

In the first version of the method, the fire scenarios to be used represented either cases where fire suppression leads to successful extinction of the fire or cases where fire suppression is not successful.

- For successful fire suppression, the scenario duration was equal to the estimated time required to detect and extinguish the fire.

The smoke produced by the fire was assumed to be cooled by indoor mixing, absorption of heat by the building and fire suppression. The maximum fire size in cases of successful suppression of the fire was assumed to be 100 m^2.

- For unsuccessful fire suppression, the scenario duration was equal to the 'initial stage' of the fire, during which the building structure would remain (largely) undamaged. The smoke produced by the fire was assumed to cool through indoor mixing and absorption of heat by the building. The 'developed stage' of the fire, with building collapse and significant plume lift-off, was assumed to start to occur after 20 or 30 minutes, depending on the fire-resisting capacity of the building. No calculations were required for the developed stage of the fire.

In 1997, the maximum fire size to be used in the risk assessment was increased to the maximum floor area of the fire compartment, ultimately being 2500 m^2. In 2009, the maximum fire size to be used was lowered to 900 m^2. In both cases, no specific studies of the building integrity or the buoyancy of the release were carried out. Plume lift-off was still assumed to be insignificant due to indoor cooling and cooling in the recirculation zone of the building.

Since 2009, the general SAFETI-NL 'Roof/Lee' building-wake model for mixing in the recirculation zone has had to be used. A consequence of using this model is that lift-off effects of the plume are ignored; the plume remains grounded, regardless of its density.

2.6.3.5 Passive dispersion

After mixing in the recirculation zone of the building, the smoke plume was assumed to disperse as a neutrally buoyant plume. Gaussian dispersion models were used to calculate the dispersion for different weather conditions. Until 2006, users could use their preferred software tools to calculate dispersion and risk. Since 2006, the use of SAFETI-NL has been obligatory. Details of the 'unified dispersion model' (UDM) in SAFETI-NL are available for SAFETI-NL users in the SAFETI-NL documentation [21].

2.7 Exposure and toxic impact

Outdoor concentrations are used to determine exposure and toxic impact. The maximum exposure duration is determined by the maximum release duration, which is 1800 s.[14]

A probit function with probit values is used to translate toxic exposure to a probability of fatality [5]. The probit values are material-specific. The probit values for HCl, NO_2 and SO_2 were derived in the 1990s [17]. Generic probit values for ADR class 6 packing group I and II materials were proposed in 2009 [5]. New probit values with a better scientific underpinning have been proposed for HCl, NO_2 and SO_2 in recent years [18]. Their use in the legally required risk calculations has not yet been approved by the relevant Ministry.

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[14] The same generic maximum release duration is also used for other activities with hazardous chemicals.

For mixtures, lethality is calculated as if the different components of the mixture were independent. For each component, the probability of survival is calculated from the toxic dose. The survival fractions are then multiplied. Though simple, this approach tends to underpredict the probability of fatality for exposure to multiple toxic substances in a mixture.

The release duration is limited to a maximum of 30 minutes. This maximum is used for all activities for which risk calculations are carried out [5]. The value was proposed during the development of the earliest calculation methods in the early 1980s and has not been modified since.

2.8 Risk and decision-making

The Dutch risk calculation method [2] prescribes the weather classes that should be used for the risk assessment. It also provides the probabilities of different wind directions per weather class.

Two different outcomes are used for decision-making and land-use planning: the individual risk contour of 10^{-6} per year and the maximum effects contour.

- The individual risk contour of 10^{-6} per year defines the zone where the presence of population should be avoided. Individual risk is defined as the probability than an individual person will die as a consequence of an industrial accident at a specific site, and is location-specific. Some conservative assumptions are used to calculate the probability of fatality.
- The maximum effects contour defines the area where additional protective measures for people within buildings should be considered. For toxic scenarios, this contour is the area where the concentration within a building can exceed the life-threatening concentration of a toxic substance, if an accident occurs.

2.8.1 Individual risk 10^{-6} per year contour

Individual risk (IR) is calculated per location and is defined as the probability that a person will die as a result of an accident if the person is permanently unprotected present at that location. IR is calculated per activity; in this case the chemical warehousing. It is the sum of the risk contributions of the different scenarios that are deemed possible for the activity. The guideline for risk calculation [2] defines which scenarios should be accounted for.

The IR 10^{-6} contour connects the locations where the calculated IR has a level of 10^{-6} per year (fatality rate 10^{-6} per year). Within the IR 10^{-6} contour, the presence of population should be avoided.

Some conservative assumptions are used to calculate the IR. For example, it is assumed that a person is continuously present at the location and that the person is unprotected. In addition, it is assumed that that person will not (or cannot) move away or shelter in the event of an accident.

Generic risk calculation parameters are defined in Module B of the guideline for risk calculation [2]. Identical values are used for all activities for which risk calculations should be carried out. An example of a generic parameter is the maximum release duration of 1800 s.

2.8.2 *Maximum effects contour*

The maximum effects contour comprises the area where people may experience serious, potentially life-threatening, harm in event of a major accident at the hazardous activity (in this case: the chemical warehousing). The maximum effects contour is the envelope of the effect contours for specific types of accidents (major and minor). Within the maximum effects contour, local public authorities should assess whether the level of risk is deemed acceptable or whether additional protective measures are required.

The guideline for risk calculation [2] defines which types of accidents (scenarios) should be included in the analysis. These scenarios are the same as those used for the IR calculation.

For toxic scenarios, serious, possibly life-threatening, harm may occur if the critical (‘life-threatening’) concentration of a toxic substance is exceeded at a location [19]. These critical concentration values are substance-specific. To determine the maximum effects contour, it is assumed that people can shelter indoors. It is thus evaluated at which locations the indoor concentration can exceed the life-threatening value.

The three toxic combustion products that are identified in the current method for chemical warehouses (HCl, NO_2 and SO_2) are assumed to have similar toxic effects. Therefore, the concentrations of these three components (in ppm) are added, and the sum is compared with the lowest critical value of the three (in this case 75 ppm). This approach is conservative.

Table 12 Life-threatening concentrations of NO_2, SO_2 and HCl [19]

Substance	**Life-threatening concentration for 30-minute exposure**
Nitrogen dioxide	75 ppm
Sulphur dioxide	112 ppm
Hydrogen chloride	152 ppm

It is assumed that indoor concentrations are a factor of 2.54 lower than outdoor concentrations.[15] An indoor concentration of 75 ppm thus corresponds to an outdoor concentration of 192 ppm. Therefore, the focus zone consists of the area where outdoor concentrations can be above 192 ppm in the event of an accident.

2.9 Software implementation

Consequence and risk are calculated using SAFETI-NL. A specific warehouse model is included in the software to calculate the risk associated with the release of toxic combustion products. The relevant

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[15] It was more practical to calculate outdoor concentrations. The equivalence is derived from the assumptions that the outdoor concentration is constant and that the toxic concentration indoors is accumulating by a fixed ventilation rate of 1 building volume per hour during a period of 30 minutes.

warehouse and storage characteristics are user input for the model. The software then identifies which fire scenarios should be used and subsequently calculates the effective combustion rate, the emission rate, mixing in the recirculation zone and downwind dispersion. A risk profile is generated from a predefined set of meteorological conditions (atmospheric stability, wind speed and wind direction).

The main user inputs to the warehouse model are:

- the overall mass in the storage, the mass fraction of hazardous materials and the average composition of the hazardous materials stored;
- the total size of the storage compartment;
- the type of fire suppression system in place;
- the fraction of flammable liquids in the storage;
- the type of closing doors (manual or automatic);
- the height, length and width of the building.

The source term for non-combusted toxic products needs to be calculated manually and added in user-defined sources in SAFETI-NL.

The frequencies and relative probabilities of different scenarios are automatically calculated from the inputs above.

Generic risk inputs are:

- the location of the warehouse and the distribution of wind conditions to be used for risk calculation;
- population data for societal risk calculation.[16]

2.9.1 *Background and justification*

Until 2006, companies were free to choose the software to be used in the risk calculation. Since 2006, the use of SAFETI-NL has been prescribed in legislation. This was done in order to ensure consistency between the calculations for different companies and warehouses. More information is provided in two papers by Uijt de Haag [22, 23].

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[16] Societal risk calculation has not been discussed in this paper, since it will no longer be required once new legislation [7] comes into effect.

3 Literature survey

3.1 Introduction

A literature survey was carried out to determine which components of the risk method might be improved using publicly available information. Around 80 possibly relevant scientific papers were found using searches in Scopus [24]. The search strings that were used are listed in Appendix 1. The titles and abstracts of these papers were used to investigate their relevance. Other relevant papers, reports and handbooks were found using internet search engines and references in the papers and reports initially found. Finally, the SFPE Handbook for Fire Protection Engineering [25] and the Enclosure Fire Dynamics Handbook by Karlsson and Quintiere [30] were scanned for relevant information.

The literature survey was focused on the following topics:

- Fire development: dynamics of and stages in the development of a warehouse fire.
- Toxicity of the plume: survival fraction of toxic products, formation of and conversion factors for toxic combustion products.
- Release and dispersion: ways in which products are released from a building, their interaction with the building, buoyancy of the plume, dispersion and downwind concentrations.

3.1.1 Assumptions and limitations

The following assumptions about warehouses and risk modelling were used to determine whether available information could be useful for the development of an improved risk calculation method:

- The dimensions of the warehouse and its fire compartments will be known.
- The type of ventilation and the ventilation rates of the fire compartments will be known.
- The type of fire suppression system that are present in the fire compartments (if any) will be known.
- A maximum amount of stored product for each fire compartment will be specified in the site permit. Maximum amounts per ADR class will also be specified in the permit. The actual amounts present will vary per day and per season. This variation can be considerable.
- Per ADR class, various products will be stored. The chemical composition and physical and chemical properties can differ substantially for products in the same ADR class.
- In a typical fire compartment, both solid and liquid products will be stored. Gases and liquefied gases will be stored in dedicated areas within the fire compartment. Liquid products are typically stored in intermediate bulk containers (IBCs) or drums. Solid products are stored in plastic or metal drums, cardboard or plastic packaging or open containers. Gases and liquefied gases are stored in gas cylinders. Steel vessels can also be used for liquids, liquefied gases and gases, but are rare.

- IBCs, drums and packages are normally placed on wooden pallets. These are placed directly on the ground, in a stack of pallets on the ground or in dedicated racks. All modes can be seen in a single fire compartment.
- If a fire is not actively suppressed, it will propagate and develop into a larger fire. Both stored products and other combustible material in the warehouse, e.g. wooden pallets and plastic material, will contribute to the fire.

3.2 Warehouse fire frequency

Warehouse fire frequency was not a specific part of this study. However, two references were found that provided figures for warehouse fire frequency.

The first reference is to a cost–benefit analysis of chemical warehouse fire compartmentation that was published in 2003 [31]. The likelihood of fire initiation is discussed in section 3.3 of that report. Four different information sources for warehouse fire frequencies were compared. The agreement between the data was found to be reasonable. According to the meta-analysis [31], the likelihood of a fire that will not self-extinguish or be immediately extinguished by people nearby is in the order of 10^{-2} per year per unit or between 1×10^{-5} and 3×10^{-5} per m^2 floor area per year. This value is more than one order of magnitude higher than the value used in the existing Dutch method (8.8×10^{-4} per unit per year).

The second study is a recent proposal for a risk calculation method for chemical warehouses by the UK Health and Safety Executive [32]. Module 10 of that study involves a frequency analysis. According to the authors, the rate of serious fires (causing widespread structural damage to the roof) is around 10^{-2} per year for a standard warehouse. For a chemical warehouse, the same fire frequency could be lower, e.g. around 3×10^{-3} per year.

3.3 Development of building fires

3.3.1 General stages of a fire

A large amount of information is available on the development of fires in general. This includes reports from research institutes on the internet, publications in journals and dedicated fire engineering handbooks such as the NFPA SFPE Handbook of Fire Protection Engineering [25]. For compartment fires, the book Enclosure Fire Dynamics [30] by Karlsson and Quintiere provides a good starting point, as it summarises the key insights and model developments until the early 21st century.

Fire development depends on the chemical and physical properties of the products contained in the fire and on building characteristics such as size, ventilation rate and storage configuration. It also depends on possible suppression of the fire by automatic systems or manual operations. Stored materials, packaging materials and construction materials all contribute to a fire and, depending on their characteristics, can either accelerate or decelerate its development. Packaging will aid fire spread if it is readily combustible and will slow fire spread when not readily combustible.

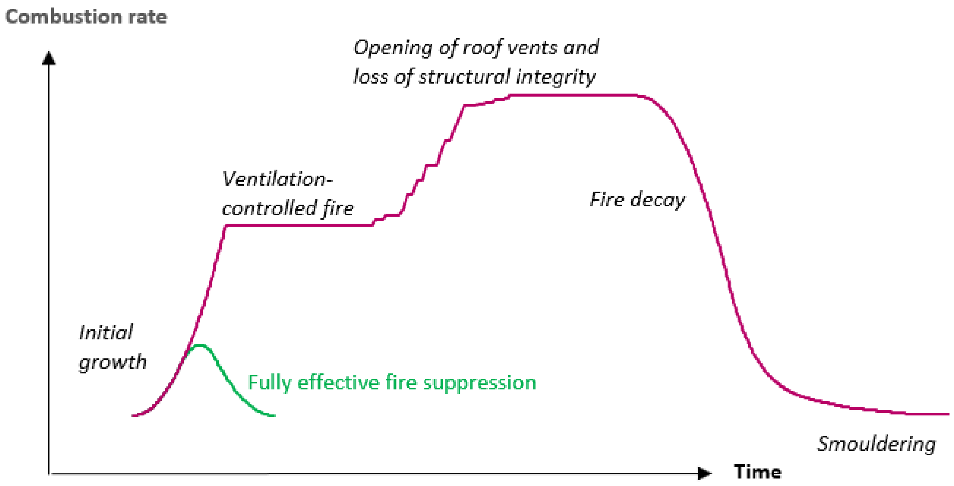

Figure 1 Development of the combustion rate over time

For a compartment fire that is not suppressed, the following stages can be distinguished: ignition, initial growth, ventilation-controlled fire, fully developed fire, decaying fire and smouldering fire. Figure 1 shows how the combustion rate develops over time.

- Ignition: The fire starts with some process that triggers chemical combustion that is sufficiently strong to propagate.
- Initial growth: The fire is still localised. The heat release grows quadratically over time. The fire growth rate is a function of fuel properties and local storage conditions. Oxygen is sufficiently available, and the combustion rate is said to be ‘fuel-controlled’.
- Ventilation-controlled fire: If the fire is not suppressed, the combustion rate will reach a temporary maximum that is determined by the oxygen supply. The fire is then said to be ‘ventilation-controlled’ or ‘oxygen-controlled’.
- Flashover: ignition of unburned flammable vapours in a hot upper gas layer of the compartment. Materials throughout the compartment are heated by radiation from the upper layer and ignite. The fire rapidly expands to the full size of the compartment. The combustion rate still depends on oxygen supply and will not increase substantially if the building structure remains undamaged. Flashover can be prevented by adequate smoke venting (as part of the design of the fire compartment).
- Fully developed fire: characterised by a large burning area, increased oxygen supply via openings in the building and a high combustion rate
- Decaying fire: The fire starts to decay when most of the fuel is consumed or has become charred.[17] The combustion rate will decrease, and the heat release will reduce.
- Smouldering fire: If solid fuels are present, the fire can smoulder for a significant amount of time. In a smouldering fire, combustion is slow and incomplete due to the lowered temperatures and degraded (charred) materials. Further

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[17] Charring is the formation of an insulating layer on the surface of a solid material. The insulating layer prevents vapours from escaping from the material.

degradation of the fuels and reduction of the fire temperature will eventually result in extinction of the fire.

Fire suppression systems should respond in the earliest stages of the fire in order to be fully effective. If so, they may be able to fully extinguish the fire. Fire suppression can also be partially effective, e.g. by limiting or delaying fire growth. The effect of partially effective fire suppression is not visualised in Figure 1; the line can be anywhere between the magenta line (zero effect of fire suppression) and the green line (full effect of fire suppression).

The following conclusions on the assessment of hazard and risk related to toxic exposure outside the warehouse can be drawn:

- The most important parameter for hazard assessment is the likelihood that fire suppression will be fully successful. Significant releases of toxic substances are expected only if fire suppression is not fully successful.
- If fire suppression fails, the emission of toxic substances depends on the combustion rate of the ventilation-controlled fire and that of the fully developed fire. The initial stage of the fire is not particularly relevant for toxic exposure outside the warehouse.

3.3.2 *Initial stage of the fire*

During the initial stage of the fire, the fire will expand and grow. The propagation speed is different in horizontal and vertical direction, and is determined by the storage configuration, fuel characteristics and possible air currents within the warehouse, among other factors.

A frequently used simplification is that the fire will initially expand radially and at constant speed. Fire area, mass combustion rate and amount of heat produced will then increase quadratically with time. Models that assume this dependency are referred to as t^2-models.

In the t^2-model, the development of the heat release rate Q can be expressed as:

$$Q(t) = \alpha \, t^2 \qquad (5)$$

where:
Q(t): the heat release rate (e.g. in kW)
α: the fire growth rate (e.g. in kW/s^2)
t: time (e.g. in s).

Appendix 1 of NFPA code 72 (see Table 13) provides ranges for α for slow, intermediate and fast fire development. Slightly different values for slow, medium, fast and ultrafast fire development are provided in a report by Kim and Lilley [33] (see Table 14). Similar values can be found in a paper by Evans [34].

Table 13 Generic fire growth rates in NFPA code 72

Fire development	**Fire growth rate (α) (kW/s²)**	**Time to reach 1 MW**
Slow	$\alpha \leq 0.0066$	≥ 390 s
Medium	$0.0066 < \alpha \leq 0.0469$	150 – 390 s
Fast	$\alpha > 0.0469$	< 150 s

Table 14 Generic fire growth rates in reference [33]

Fire development	**Fire growth rate (α) (kW/s²)**	**Time to reach 1 MW**
Slow	$\alpha = 0.0028$	600 s
Medium	$\alpha = 0.0111$	300 s
Fast	$\alpha = 0.0444$	150 s
Ultrafast	$\alpha = 0.1778$	75 s

The t^2-growth assumption is valid when the following conditions are met:

- Fire spread is two-dimensional.
- The fuel and storage characteristics are largely homogeneous within the fire area.
- Oxygen supply is not a limiting factor.
- The maximum fire size has not yet been reached and flashover has not yet occurred.
- There is no (effective) suppression of the fire.

The fire growth rate α depends on the storage configuration and fuel characteristics. Specific values for specific materials can be found in fire prevention handbooks such as [25] and [30] and in dedicated studies such as [33]. Hurley and Bukowski have noted that these values should be used with care, as they are valid only for specific conditions and circumstances [35]. In addition, most data relate to fires fuelled by furniture such as wooden chairs, plywood wardrobes and mattresses. As a result, these data have little relevance to chemical warehouses containing different types of liquids and solids in packages and possibly stacked in racks.

The UK Health and Safety Executive (HSE) has provided heat release rates per unit area (MW/m²) and fire growth rates (kW/s²) for different paper, wood and plastic products and for different stack heights [36]. These data show that the fire growth rate can increase substantially as the stack height is increased (see table 2 in [36]).

Fire growth parameters for building fires are discussed in a paper by Holborn, Nolan and Golt [37]. The authors used a dataset of 2500 fire accidents that occurred in buildings in London between 1996 and 2000. This set also contains 20 fires that were classified as warehouse fires (general warehouse fires; not necessarily chemical warehouse fires). The fire growth rate for the different types of buildings was estimated from a least-squares fit of the fire growth between detection and time of arrival of the fire brigade. Compared with fires in other types of buildings, warehouse fires have a faster growth rate and result in larger fires. According to Holborn, Nolan and Golt, these 'structures often present a large undivided space for a fire to spread through. The involvement of sandwich panel cladding and fuel sources with a fast heat release rate (e.g. plastics) were also found to be important contributing factors in several cases.' The resulting estimate for the growth rate of warehouse fires was 0.107 kW/s^2. Given the diversity of warehouses and warehouse fires, this number should be used with prudence.

For storage in racks, the assumption that fire spread is two-dimensional does not apply to the initial stage of the fire. Yu has proposed a t^3-dependence [38]. A more complex correlation has been proposed by Ingason [39].[18] Once the fire has progressed to multiple racks, further fire spread will become two-dimensional by approximation.

3.3.3 *Fuel-controlled fire*

In the absence of effective fire suppression, the fire will continue to grow. Initially, enough oxygen is available for combustion and the fire is said to be 'fuel-controlled'. During this stage, the combustion process is relatively efficient, and the fire temperature is relatively high.

Typical combustion rates per unit area (kg/s·m^2) for different materials can be found in fire prevention handbooks such as [25] and [30]. Most organic liquids have a combustion rate per unit area between 0.05 and 0.1 kg/m^2·s, while common organic solids and plastics typically have a combustion rate per unit area between 0.01 and 0.05 kg/m^2·s [30].

Further points of interest:
- If products are stored in high racks, it must be checked whether the values reported in the literature are indeed applicable to this storage height.
- The effect of packaging materials on the overall combustion rate should also be considered.

3.3.4 *Ventilation-controlled fire*

At some point, oxygen supply can become a limiting factor for further growth of the fire. The fire will then become 'ventilation-controlled'. The extent of the fire may still increase, but the overall combustion rate (kg/s) is capped by the (limited) availability of oxygen. According to the HSE, a rapidly growing fire in a relatively small storage space may become ventilation-controlled within a few minutes, while for slowly developing fires in large buildings the transition to ventilation-controlled burning may take many tens of minutes [36]. In extreme cases, ventilation-controlled burning may not occur at all.

In deficit of oxygen, the combustion rate is determined by the availability of oxygen. The oxygen demand of the fire can be derived from the chemical composition of the fuels and presuming stoichiometric combustion. Oxygen can be supplied to the fire by active ventilation or via openings in the building (natural ventilation).
- Active ventilation: The oxygen supply can be determined from the mechanical ventilation rate that is set for the ventilation system.
- Natural ventilation: In the early stage of a fire, the impact of the fire on the ventilation is limited and the ventilation is 'wind-driven'. As the fire progresses, hot fumes accumulate in the

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[18] $Q_c = H \cdot \alpha \cdot e^{\beta t} \cdot (a + b \cdot t)$. In this correlation, $Q_c(t)$ is the convective heat release rate, H the stack height t time (in s) and α, β, a and t fitting parameters that should be determined from experimental data.

building. As a result, the pressure difference across the openings and the corresponding ventilation rate increase. This regime is called 'buoyancy-controlled ventilation'.

For buoyancy-controlled ventilation, the air mass flow rate is assumed to correlate with the 'ventilation factor' $A_0\sqrt{H_0}$ [29]:

$$\dot{m}_a = c\, A_0 \sqrt{H_0} \qquad (6)$$

where:
$\dot{m}_a$: the air mass flow rate, in kg/s
c: the ventilation constant, in kg/s·$m^{5/2}$
A_0: the area of the opening, in m^2
H_0: the height of the opening, in m.

A value of 0.5 is commonly used in the literature for the ventilation constant (e.g. [29], [30], [40]). According to [30], this approximation is applicable when the compartment is well mixed, the indoor temperature exceeds 300 °C and the production rate of combustion gases is negligible compared with the air inflow rate. More details on buoyancy-controlled flow from a vent can be found in chapter 5 of [30].

Once the air mass flow is known, the combustion rate can be estimated from the assumption that the combustion is stoichiometric [40]:

$$\dot{m} = \frac{0.5}{r} \cdot A_0 \cdot \sqrt{H_0} \qquad (7)$$

where:
$\dot{m}$: the combustion rate in kg/s
r: the stoichiometric air-fuel mass ratio.[19]

3.3.5 *Flashover*

In a fire, non-combusted vapours are released. These vapours accumulate near the top of the warehouse due to their high temperatures. The mixture of non-combusted vapours and air can ignite if the fraction of non-combusted vapours in the upper smoke layer is high enough and if the temperature of the upper smoke layer is above the self-ignition temperature of the mixture.[20] Ignition of the upper smoke layer in a building is called flashover.

Flashover results in rapid heating of the remaining material in the warehouse and rapid expansion of the fire. Shortly after flashover, the entire warehouse can be on fire. As long as the building is largely undamaged, the combustion rate is governed by the oxygen supply.

Roof vents can prevent flashover if adequately designed, installed and maintained in a good condition.

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[19] Mass of air required for combustion divided by fuel mass.

[20] The self-ignition temperature of the vapours in the upper smoke layer is generally believed to be somewhere between 500 and 600 °C [30].

3.3.6 *Loss of structural integrity*

The building structure will lose strength as it is heated by the fire. If the temperature is high enough, plastic sheets and roof lights can burst and cracks in walls and roofs may appear. If the temperature further increases, the building or its roof can collapse due to loss of strength of the supporting structures.

Fire compartments in chemical warehouses in the Netherlands normally have a designed fire resistance of 60 minutes. The building structure should remain undamaged during this period. Maintaining the designed fire resistance during the lifetime of a building can be a challenge. A fire resistance of 60 minutes is not required if the fire compartment is isolated from other structures.

More information on material responses to increased temperature, including critical temperatures for different types of steel, can be found in section 1, chapter 10 of the SFPE-NFPA Handbook of Fire Protection Engineering [27].

If parts of the building structure fail, more oxygen can be fed to the fire. The combustion rate will subsequently increase. In abundance of oxygen, the fire will once again be fuel-controlled, with a corresponding combustion rate.

3.3.7 *Fire decay*

When most fuel is consumed, the combustion rate will decrease, and both the heat release and the temperature of the fire will reduce. This could result in a smouldering fire, where combustion is slow and incomplete due to the lowered temperatures. A commonly used assumption is that fire decay is proportional to t^{-2} [41].

3.3.8 *Effect of packaging on fire spread*

Hazardous substances in warehouses are normally stored in packaging such as metal or plastic drums, cardboard boxes or sacks, or plastic IBCs. Drums and boxes can be packed together in plastic and stored on pallets.

The effect of packaging on warehouse fire spread is discussed in a report by Hietaniemi and Mikkola [42]. In general:

- Packaging can increase fire spread if the packaging material is readily combustible.
- Packaging can reduce fire spread if it is not readily combustible.
- Upon failure, packaging contaminates the stored product and the combustion characteristics of the mix will differ from those of the stored products alone.

Further details for plastic containers, metal containers and paper and cardboard boxes and sacks are given in section 3.2 of [42]. Not surprisingly, metal containers provide the greatest resistance to fire and paper and carboard boxes and sacks the least.

3.3.9 *Effect of storage in racks on fire spread*

Rack storage fires are discussed in research reports by Ingason [39] and Lönnermark and Ingason [43]. Medium- and large-scale tests were carried out to measure the heat release rate of fires in racks that were filled with cardboard boxes. The storage height, the spacing between the racks and the contents of the boxes were varied between the tests. According to [39], the greatest height of the racks used in these experiments was 5.2 m.

Once goods have caught fire, flames first spread upward in the rack and subsequently horizontally towards other racks. Figure 4.5 in [43] shows how a fire can progress from one rack to another. Not surprisingly, the distance between the racks proved to be an important parameter for fire propagation. Other important parameters were the vertical spacing between the top of the rack and the ceiling, the rack height and the contents of the boxes.

3.3.10 Effect of storage of general goods in the compartment

Before 2016, hazardous substances should be stored in dedicated fire compartments and general trade goods should not be stored in these dedicated compartments. Since 2016, both general trade goods and hazardous substances can be stored in the same fire compartment [10], provided that the ignition probability and the fire growth rate are not substantially increased, and that the effectiveness of suppression systems is not substantially reduced.

A reviewer of this report expressed specific concerns about Li-ion batteries stored in a fire compartment, as a significant amount of heat can be released when Li-ion batteries catch fire. In addition, hydrogen fluoride (HF) can be released. The impact of storing both hazardous substances and Li-ion batteries in the same fire compartment has, however, not yet been investigated.

3.3.11 Effect of fire suppression

Fire suppression systems are intended to either extinguish a fire or limit its growth. The effect of suppression systems can be characterised by their response time and the subsequent response of the fire suppression system. For all cases, the design of the suppression system should be such that at least flashover is averted.

Fire suppression systems can fail to respond at all or respond too late or too little, i.e. fail to control the fire within designed safe limits. As a simplification, the following three responses are distinguished:
- Fully effective: The suppression system is successful in controlling the fire; the fire is either rapidly extinguished or its size is kept within designed safe limits.
- Failure: The suppression system fails to control the fire within safe limits. Due to the ineffective response, further growth of the fire and eventual flashover cannot be prevented.
- Partial failure: The suppression system fails to extinguish the fire or keep the fire size within designed safe limits but does limit the combustion rate and prevent flashover.

3.4 Quantities for hazard assessment

3.4.1 Combustion rate

Fire models are most often used to predict fire propagation to adjacent compartments and buildings or to assess the effect of fire mitigation systems. For these uses, the heat release rate (Q) is more important than the combustion rate ($\dot{m}$). Therefore, fire development is normally expressed in terms of the heat release rate. As the heat release rate depends only on the combustion rate and the effective heat of combustion (H_{eff}), a conversion between the two is relatively simple.

$$\dot{m} = \frac{Q}{H_{\mathrm{eff}}} \tag{8}$$

where:
$\dot{m}$: the combustion rate in kg/s
Q: the heat release rate in kW
H_{eff}: the effective heat of combustion per unit mass, in kJ/kg.

The effective heat of combustion is further discussed in Section 3.4.2.

The development of the combustion rate was summarised in Section 3.3.1 and Figure 1.

- Initially, the combustion rate will grow with t^2.[21]
- If the fire is not suppressed, it will continue to grow until oxygen supply becomes a limiting factor. The fire is then said to be 'ventilation-controlled'.
- Flashover will not significantly increase the combustion rate if the oxygen supply is not increased.
- The combustion rate further increases once the building structure starts to fail, due to the enhanced oxygen supply.
- The combustion rate will decay once most of the fuel is either consumed or charred (limiting the release of combustible gases).
- Fire suppression systems are designed to prevent flashover. Their activation should be during the initial growth stage. If the suppression system is fully effective, the fire will normally be extinguished rapidly after its activation. If the fire suppression partly fails, its effect can vary from practically zero to almost fully effective.

3.4.2 *Energy production*

The heat release rate is the product of the effective heat of combustion of the fuel and the combustion rate, see equation 8. The effective heat of combustion is the product of the combustion efficiency (χ_{eff}) and the ideal heat of combustion (equation 9).

$$H_{\mathrm{eff}} = \chi_{\mathrm{eff}} \cdot H_{\mathrm{c}} \tag{9}$$

The ideal (or complete) combustion energy of a material is the energy that is produced if combustion of the material is complete. Assuming constant pressure, the ideal combustion energy of a material is equal to the difference in the formation enthalpies of the materials before and after the reaction. For organic flammable liquids and gases, the ideal heat of combustion is normally between 30 and 50 MJ/kg. Wood and plastic are normally somewhere between 15 and 30 MJ/kg (see e.g. table 1-5.3 in [26]). In real fires, combustion is incomplete because the

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[21] Generic growth rates for the heat release rate can be found in Section 3.3.2.

temperature and oxygen concentration in a real fire will deviate from the ideal circumstances for combustion.
The effective heat of combustion is the nett amount of heat released by the combustion. It takes into account that actual combustion is incomplete. While the complete heat of combustion is constant, the effective heat of combustion depends on temperature, availability of oxygen and material conditions.

The combustion efficiency is the ratio between the effective and ideal heat of combustion ($\chi_{eff} = H_{eff}/H_c$). The combustion efficiency depends on the temperature, the amount of oxygen available to the fire, the presence of halogens in the fuel mix and, in the case of solid fuels, their state (charred or not). Values for combustion efficiency can be found in the literature:

- According to Drysdale [26], combustion efficiency roughly varies between 0.3 and 0.9. The lower value pertains to heavily fire-retarded materials, the upper value to materials that contain enough oxygen in their molecular structure to sustain combustion.
- In a paper by Purser [46], combustion efficiency is plotted against the equivalence ratio[22] for a dozen different materials. On average, combustion efficiency reduces linearly with the equivalence ratio, starting from 1 for an equivalence ratio equal to 0.5 and ending at 0.3 for an equivalence ratio equal to 3. Polyvinylchloride (PVC) is known to have a very low combustion efficiency due to the high amount of chlorine (a halogen) in this material.
- Combustion efficiencies for specific rack storage fires were reported by Ingason [39]. The reported efficiencies depend on the spacing between adjacent boxes in a rack. With little spacing, combustion efficiency reduces to 0.25. With substantial spacing, the efficiency increases to 0.75. The most likely explanation is that combustion becomes less efficient with small spacing due to limited oxygen supply.

Another method of calculating the energy produced in a fire is to assume a correlation between the heat release and the air mass inflow rate. According to Watson and Thomas, the heat release per mass of air consumed is approximately 3 MJ/kg for most fuels [29].[23] For oxygen supply via openings in the building, the air mass intake can be calculated using equation 6. For active ventilation of the building, the air supply can be derived from the ventilation rate.

3.4.3 *Energy transfer*

The produced heat is transferred to the environment by convection, radiation and conduction. Conductive heat transfer is usually small compared with convective and radiative heat transfer.

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[22] The equivalence ratio is the quotient of the amount of air needed for combustion and the amount of air available for combustion.

[23] According to [30], the heat release rate is typically 13.1 MJ per kg of oxygen consumed. This value is equivalent to 2.8 MJ/kg of air and should be accurate within 5% for most hydrocarbon materials.

The convective heat fraction (χ_{conv}) is defined as the fraction of the ideal heat of combustion (H_c) that is transformed into convective energy (H_{conv}):[24]

$$\chi_{\text{conv}} = \frac{H_{\text{conv}}}{H_{\text{c}}} \tag{10}$$

Likewise, the radiative heat fraction (χ_{rad}) is defined as the fraction of the ideal heat of combustion (H_c) that is transformed into radiative energy (H_{rad}):

$$\chi_{\text{rad}} = \frac{H_{\text{rad}}}{H_{\text{c}}} \tag{11}$$

If conductive energy can be ignored, the sum of the two energy fractions is equal to the combustion efficiency:

$$\chi_{\text{eff}} = \chi_{\text{rad}} + \chi_{\text{conv}} \tag{12}$$

The radiative and convective energy fractions depend on the amount of oxygen available. Detailed data for specific materials can be found in table 3-4.15 of [28]. Table 15 provides a summary of fire characteristics for well-ventilated fires in the absence of heat losses to the building. For under-ventilated fires, the combustion efficiency will be lower. As a result, χ_{conv} and χ_{rad} will also be lower.

Table 15 Combustion characteristics for different types of materials for well-ventilated fires in the absence of heat losses to the building (derived from Table 3-4.15 in [28])

Type of material	**Average heat of combustion (MJ/kg)**	**Average combustion efficiency**	**Average χ_{conv}**	**Average χ_{rad}**
Common gases(a)	47	0.89	0.60	0.29
Common liquids(b)	35	0.83	0.56	0.29
Chemicals and solvents(c)	24	0.67	0.49	0.28
Pesticides(d)	14	0.52		
Wood(e)	17	0.74	0.48	0.26
Solid synthetic materials(f)	27	0.64	0.36	0.32

(a) Derived from data for 6 common flammable gases.

(b) The average heat of combustion and average combustion efficiency were derived from data for 15 common flammable liquids. The convective and radiative heat fractions were derived from 13 of these flammable liquids. As a result, the sum of the convective and radiative heat fractions is not equal to the combustion efficiency.

(c) The average heat of combustion and average combustion efficiency were derived from data for 23 chemical solvents. The convective and radiative heat fractions were derived from 15 of these solvents. As a result, the sum of the convective and radiative heat fractions is not equal to the combustion efficiency.

(d) The average heat of combustion and average combustion efficiency were derived from data for 5 pesticides.

(e) Derived from data for 3 different types of wood.

(f) The average heat of combustion and average combustion efficiency were derived from data for 41 solid synthetic materials. The convective and radiative heat fractions were derived from 31 of these solvents. As a result, the sum of the convective and radiative heat fractions is not equal to the combustion efficiency.

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[24] See for example Section 3 Chapter 4 of the SFPE Handbook of Fire Protection Engineering [28].

The data presented in Table 15 do not take into consideration heat losses to the building. For fires within buildings, most of the radiated heat is consumed by the building structure and flooring materials. A small fraction of the radiated heat is absorbed by the air and smoke in the building. The convective heat generated in the combustion process (within the building) is largely preserved by the (hot) gases in the building. Nevertheless, a small fraction of this convective heat can be absorbed by the building structure. According to the HSE [36], the proportion of the heat released that is lost to the building structure ('fabric of the building') depends on the fire stage:

- In the early stages of a fire, at least 90% may be transferred to the building structure.
- When the fire becomes ventilation-controlled, the fraction of heat lost to the building may be in the order of 60–90%.
- After roof collapse, the proportion of heat lost to the building is assumed to reduce to values below 30%.

3.4.4 *Indoor temperature*

Initially, the fire size will be limited. The temperature in the compartment will be highest in and just above the combustion zone. Just above the combustion zone, the temperature will normally be between 300 and 600 ^{0}C. Hot combustion gases rise from the combustion zone and accumulate under the roof. The temperature and depth of this layer increase with time. Away from the combustion zone and away from the roof, the temperature will not increase substantially as long as the fire remains localised.

Flashover can occur if the temperature of gases under the roof has increased to around 500 or 600 ^{0}C [30]. After flashover, the fire will no longer be localised, and the production of smoke and heat will increase significantly. Temperatures will be high throughout the compartment, typically between 600 and 1000 ^{0}C.

Lower temperatures apply to smouldering fires. For this type of fire, the temperature of the hot gas layer under the roof is assumed to be between 25 and 85 ^{0}C [48].

3.4.5 *Smoke composition: conversion factors and survival fraction*

Both toxic combustion products and non-combusted toxic materials in the smoke plume contribute to its toxicity. A full survey of available information on toxic products was outside the scope of this study. Detailed information on the toxicity of smoke plumes can be found, for example, in the handbook Fire Toxicity [47] and in a paper by Purser [46].

The amount of non-combusted toxic material in the smoke depends on the 'survival fraction' of the toxic material stored in the warehouse. This parameter describes how much product is vaporised and lifted and dragged into the smoke plume without combusting. According to the HSE, medium- and large-scale tests performed by the Health and Safety Laboratory showed that the maximum survival fraction is around 30% [51]. This maximum applies to toxic materials stored in the upper parts of a high rack system that are engulfed in a fire from below. A value of 10% was assumed to be a reasonable upper limit for high-rack storage, while lower values would be applicable for low-level storage of toxic materials and for pool fires.

The formation of toxic combustion products depends on the molecular composition of the fuels and on the completeness of the chemical reactions in the fire zone. The latter is very temperature dependent. A good overview of the relevant parameters is provided in a paper by Purser on toxic yields and mass release rates [46].

- The mass loss yield of a toxic combustion product p (y_{p}) is defined as the fraction of the toxic mass production rate of that component ($\dot{m}_{\mathrm{p}}$) and the combustion rate ($\dot{m}$).

$$y_{\mathrm{p}} = \frac{\dot{m}_{\mathrm{p}}}{\dot{m}} \tag{13}$$

- The recovery fraction (also known as conversion efficiency or conversion factor) of a toxic combustion product is the fraction of the obtained mass yield of that component ($\dot{m}_{\mathrm{p}}$) and the maximum possible yield of that component ($\dot{m}_{\mathrm{p,max}}$). For example, the recovery fraction of CO is the fraction of CO that is actually produced plus the amount of CO that would have been produced if all carbon in the fuel had been converted into CO.

$$R_{\mathrm{p}} = \frac{\dot{m}_{\mathrm{p}}}{\dot{m}_{\mathrm{p,max}}} \tag{14}$$

In Purser's paper [46], toxic yields for well-ventilated conditions and under-ventilated conditions are provided for 13 different polymers. The same publication also contains a plot for the CO recovery fraction as a function of the equivalence ratio. In excess of air (equivalence ratio below 1), the CO recovery fraction is below 0.05 for most materials. In deficit of air, the recovery fraction increases to values between 0.05 and 0.3, depending on the type of material. According to Purser, the recovery fraction is particularly sensitive to the amount of halogen/flame-retardant in the fuel. Halogens reduce combustion efficiency and increase the formation of only partly oxidised combustion products.

3.4.6 *Warehouse material composition*

The composition of the materials in the chemical warehouse is important in determining which toxic products can be released in what quantities. According to the guideline for risk calculations [5], the producer of the risk calculation must specify which products can be stored in the warehouse. The current subsection discusses the information about the composition of materials in chemical warehouses that was found in the literature. This information is for reference only.

Several studies were found in which the average composition of warehouse materials was investigated:

- In the first version of the Dutch risk calculation method for warehouse fires [3], an average composition was derived from the 25 most widely sold pesticides:
  - The average molecular composition was $C_{3.6}H_{5.3}O_{0.4}N_{0.9}S_{1.3}Cl_{0.8}$.
  - The mean molecular weight (M_W) was 163 kg/kmol.

    - The active mass fraction[25] was 28%.
- In appendix 5 of the research report underlying the first version of the Dutch risk calculation method [11], compositions were derived for different substance categories:
    - Category 0: substances that produce toxic combustion products in a fire, excluding highly toxic substances (category 1):
        - Average material composition: $C_{8.23}H_{10.18}O_{1.61}N_{1.24}P_{0.03}S_{1}Cl_{0.83}Br_{0.07}Sn_{0.033}Mn_{0.04}Zn_{0.08}$.
        - Average molecular weight: 250.4 kg/kmol.
        - Active mass fraction: 53%.
    - Category 1: highly toxic substances[26]:
        - Average material composition: $C_{9.82}H_{11.49}O_{4.46}N_{1.68}P_{0.16}S_{0.13}Cl_{0.37}$.
        - Average molecular weight: 250.4 kg/kmol.
        - Active mass fraction: 28%.
    - Category 2: substances that produce either polychlorinated dibenzo-para-dioxins (PCDD) or polychlorinated dibenzofurans (PCDF) in a fire:
        - Average material composition: $C_{6.99}H_{3.14}O_{1.49}P_{0.16}Cl_{4.67}$.
        - Average molecular weight: 281.5 kg/kmol.
        - Active mass fraction: 68%.
- In the 1997 update of the risk calculation method [4], the following composition was provided as an example:
        - Average material composition: $C_{3.28}H_{4.35}O_{1.38}Cl_{1.10}N_{0.23}S_{0.06}$.
        - Average molecular weight: 101.1 kg/kmol.
        - Active mass fraction: 100%.
- In the 2009 update of the risk calculation method [5], yet another average composition was proposed, based on a new investigation carried out by the engineering company Tebodin:
        - Average material composition: $C_{3.90}H_{8.50}O_{1.06}N_{1.17}S_{0.51}P_{1.35}Cl_{0.46}$.
        - Average molecular weight: 163 kg/kmol.
        - Active mass fraction: 100%.
- According to [52], an analysis of 60 common agrochemicals gave the following average warehouse material composition:
        - $C_{22}H_{22}Cl_{2.83}N_{2.73}S_{1}O_{4.46}$.

To summarise, for these supposedly typical (agro)chemicals:

- The mass fraction of nitrogen varies from 0 to 10%.
- The mass fraction of chlorine varies from 5% to 60%.
- The mass fraction of bromine varies from 0 to 2%.
- The mass fraction of sulphur varies from 0 to 25%.
- The average weight varies from 110 g/mol to 530 g/mol.
- The average molecular weight of the combustion products varies between 35 and 42 g/mol. If mixing-in of nitrogen is considered, the average molecular weight of the combined smoke–nitrogen mixture reduces to a value between 29 and 32 g/mol (average value 30 g/mol).

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[25] All materials that combust should be considered when determining the average material composition. The active mass fraction is the mass fraction of the products that produce toxic combustion gases. Packaging material, non-hazardous solvents, inert formulations in powders, etc. are not assumed to produce toxic gases and are therefore regarded as non-active mass.

[26] 'Highly toxic' substances were defined as those with an LD50 (oral, rat) value of 25 mg/kg or less.

3.4.7 *Likelihood of effective fire suppression*

In a research report by WS Atkins Consultants on behalf of the HSE [31], the likelihood of effective fire suppression was modelled using a fault tree. Probabilities were proposed for each branch in that fault tree. The focus of the report was the likelihood of the fire spreading to adjacent compartments. This requires successful detection and successful mitigation.

- It is assumed that significant fire spread can be prevented only if the fire is detected in an early stage. In the event of early detection, automatic fire suppression or manual fire suppression by on-site personnel can be successful. In the absence of early fire detection, automatic and manual suppression are unlikely to be successful.
- Fire brigades normally arrive when the fire has already increased significantly in size. Their purpose is to prevent fire spread to adjacent compartments.
- The likelihood of successful fire detection in an early stage is discussed in section 4.2 of [31]. The work distinguishes between different types of fuels and different types of detection. For combined manual and automatic fire detection, the likelihood of successful early fire detection is assumed to be between 0.82 and 0.86.
- The likelihood of successful fire suppression (assuming early detection) is discussed in section 4.3 (automatic suppression systems) and 4.4 (manual fire suppression) of [31]. For automatic sprinklers, the likelihood is assumed to be between 0.6 and 0.9, depending on the fuel type. For automatic foam systems and automatic gas extinguishing systems, the likelihood is assumed to be between 0.8 and 0.95, depending on the type of fuel and assuming that the suppression system is suited to the fuel composition. The likelihood of successful manual fire extinction is much lower: between 0.1 and 0.4, depending on the type of fuel.

Given these numbers, the total likelihood that a fire will successfully be extinguished in an early stage is between 49% and 77% when using automatic sprinkler systems and between 66% and 82% when using automatic foam or gas systems. Thus, in the remaining cases (23% to 51% for automatic sprinklers and 18% to 34% for automatic or gas systems), successful early fire suppression is unlikely, and further efforts should focus on preventing fire spread to adjacent compartments.

Several other references were found that discuss the causes of failure and their frequencies for different types of repressions system. For example, the effectiveness of automatic sprinkler systems was reviewed by Frank et al. [44] and by Malm and Pettersson [45]. Both studies were, however, not specific to warehouses.

- Both studies highlighted differences in the definition of ‘success’ between different available information sources, e.g. either containing the fire to the room of origin or preventing significant damage to structure and property. These differences make it difficult to provide a reliable estimate for successful fire suppression by automatic sprinkler systems.

- Both studies identified the main causes of automatic sprinkler system failure.
- In [44], 'success' was defined as meeting the design requirements of the automatic sprinkler system. Fault tree analysis and fire incident data analysis were used to estimate the effectiveness of these systems. Overall, the likelihood of successful activation and response was estimated to be between 70% and 99.5%, with a peak between 90% and 95%.
- According to [45], the reliability of automatic sprinkler systems is often assumed to be around 90%. Of 66 fires in Swedish industries, 42 (64%) were successfully extinguished. In 21 incidents (32%), the fire was successfully contained (but not extinguished). In the remaining 3 incidents (5%), the fire was not successfully extinguished or contained. Further incident data from Finland, Norway, London (UK) and New Zealand, also discussed in this review, were found to slightly deviate from the numbers for Swedish industries.

3.5 Release and dispersion

3.5.1 Introduction

The dispersion of hazardous substances depends on:

- the release characteristics — in particular the volume, velocity and temperature of the emitted smoke;
- the release location and distribution, e.g. from a single opening or from multiple openings, from the top or side of the building;
- the building size, aspect ratio and orientation to the wind;
- the atmospheric stability, wind speed and surface roughness.[27]

Two features are key for dispersion:

- Mixing in the building wake: The wind flow around a building will create vortices at the sides of the building. Part of the air can be 'captured' in the recirculation zone on the downwind side of the building; the building wake. Emissions from the building can also be captured in the building wake if they do not have enough momentum or buoyancy to escape the wake. The size of the building wake depends on the length, width and height of the building. Mixing in the building wake may have opposing effects. On the one hand, the smoke plume will be diluted, creating lower concentrations in the near field when compared to open fires. On the other hand, the smoke plume will cool by mixing, thereby reducing possible plume rise and increasing ground concentrations downwind.
- Plume rise: One of the most prominent features of the smoke released from the building is its high temperature, as a result of which the release tends to be buoyant. Buoyancy can have a significant effect on ground concentrations downwind of the release. The buoyant dispersion behaviour of the plume depends on the temperature and volume of the release, weather conditions and interactions with the building. The higher the temperature and volume of the release, the more the plume tends to rise. Buoyancy effects are stronger if the wind is weak (low wind speed) and the atmosphere stable. Strong winds and

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[27] Dry deposition and wash-out are normally not considered as relevant.

atmospheric mixing suppress and reduce plume rise. Mixing of the plume in the recirculation zone (building wake) also reduces the buoyancy of the plume.

In the far field, smoke dispersion depends on atmospheric stability, wind speed and land use. For this stage of the dispersion, Gaussian dispersion models can be used. A simplified method to take the influence of land use into account is to assume an appropriate average surface roughness for the environment.

Only few literature sources were found that address the release and dispersion of fire smoke plumes from buildings specifically. A model and literature review carried out by Hall and Spanton in 2005 [53] is the most detailed and complete description of the topic to date. Most other publications have a narrower scope. For example, they describe the release of smoke from a building (not dispersion), the dispersion of ordinary emissions from a building (not fires) or the dispersion from open fires (not within buildings).

3.5.2 *Size of the recirculation zone*

The size of the recirculation zone (building wake) has not been studied in detail. Its size is normally assumed to depend on the width and height of the building; the higher these values, the larger the recirculation zone. Different models use different formulas to calculate the size of the recirculation zone. The more advanced models can differentiate between a fraction of the emission that is captured in the recirculation zone and a fraction that is not captured in the recirculation zone.

3.5.3 *Ventilation from the building*

In the early stage of a fire, the building structure will remain largely intact. Combustion gases are ventilated either by a mechanical ventilation system, if present, or by natural ventilation. As discussed in Section 3.3.4, natural ventilation is dominated by the wind if the temperature inside the building is limited, and dominated by buoyancy if the indoor temperature is sufficiently high. More details can be found in section 4.3 of [49], including the critical wind speed (or critical indoor temperature) that divides the two regimes.

As the fire further develops, windows and skylights (both often plastic) can fail and cracks or openings in constructions (in particular synthetic, steel plate or composite constructions) can occur as a result of thermal stress. In this stage, the ventilation will be buoyancy-controlled, and the ventilation rate can be derived from the size of the openings (see equation 6 in Section 3.3.4).

Eventually, the roof may collapse, resulting in a release of smoke from an open shell.

Hall and Spanton [53] distinguish four stages in warehouse fire emissions. This distinction applies to warehouses that are not actively ventilated and that do not require an outside air supply for fire suppression[28].

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[28] Such as automatic hi-ex foam installations with outside air.

- 1st stage: relatively small fuel-controlled fire with some emission of contaminants through existing cracks and faults in the structure.
- 2nd stage: initial structural damage and collapse of (e.g.) plastic lighting panels and roof lights. Increased ventilation rate, oxygen supply, combustion rate, temperature and contaminant discharge.
- 3rd stage: substantial structural damage and roof collapse. Large increase of oxygen and very high combustion rate, heat release and contaminant discharge. Unobstructed release of contaminants from building shell.
- 4th stage: fading fire. Low combustion rate and temperature. The combustion rate is low because most of the fuel has been consumed. The fire continues to smoulder. The low temperature causes incomplete combustion. The amount of contaminants in the smoke is high.

Some useful practical numbers for different types of ventilation were found in the documentation for the Firepest II software code [54]. The precise origin of these numbers (see Table 16) is unknown.

Table 16 Mass fluxes and outflow temperatures for different types of ventilation (source: [54])

Type of ventilation	**Mass flux per unit area of openings**	**Average outflow temperature**
Natural ventilation	3 kg/s·m^2	To be calculated
Failed plastic skylights	5 kg/s·m^2	120 ºC
Open smoke vents	5 kg/s·m^2	120 ºC
Small breaches in the roof	8 kg/s·m^2	200 ºC
Collapsed roof	8 kg/s·m^2	200 ºC

Hall and Spanton also emphasise the relevance of a release being distributed across the building or not. All other parameters being identical, plume rise can be very different depending on whether the release is from a single opening or from several openings across the building. This aspect is further discussed in Section 3.5.5.

3.5.4 *Terminology used to define buoyancy*

Dispersion depends on the buoyancy and the momentum of the release. In this subsection, the most important buoyancy terms will be presented, in order to facilitate further discussion later in this chapter. The terms related to momentum are not discussed, as release momentum is expected to be less relevant for the fire scenarios considered.[29] More detailed information, also including considerations of the release momentum, can be found in the literature review reports of Hall and Spanton [53] and Ramsdale and Tickle [55].

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[29] Horizontal momentum creates increased mixing near the source. This effect could be relevant for ground-level concentrations in the near field (e.g. up to 10 m) but becomes less relevant at greater distances. Vertical momentum gives higher plume heights and lower ground-level concentrations. Not considering release momentum is therefore considered to be a conservative approach. Taking momentum into consideration would complicate the analysis, as it depends on the number and size of openings and their location (in the side of the building or the roof, or both).

The first frequently used term in the literature is the lift-off parameter, L_p. The aim of this parameter is to identify when buoyant plumes would lift off from the ground. The parameter was proposed by Briggs in 1973 and was defined as:

$$L_p = \frac{g\,h\,\Delta\rho\,/\rho_a}{u_*^2} \qquad (15)$$

where:

g: the gravitational acceleration, in m/s^2
$\Delta\rho$: the density difference between ambient air and the plume, in kg/m^3
ρ_a: the ambient air density, in kg/m^3
h: a height related to the depth of the plume, in m
u_*: the atmospheric friction velocity, in m/s.

According to Hanna, Briggs and Chang [59], the parameter should be regarded as (the square of) the ratio of the internal buoyant velocity of the plume and an external mixing velocity due to atmospheric turbulence.

Several attempts have been made since 1973 to identify when lift-off starts to occur. These attempts are discussed in the 1995 report of Hall [49] and in the review report of Ramsdale and Tickle [55]. The corresponding value of the lift-off parameter was referred to as the critical L_p value. According to these authors, Briggs eventually suggested that the critical value for L_p should be somewhere between 20 and 30.[30] There was, however, no clear-cut division between plumes that lift off from the ground and plumes that do not.

A second approach is to describe buoyant behaviour in terms of the dimensionless buoyancy flux F^*. The dimensionless buoyancy flux is defined as:

$$F^* = \frac{F}{u_{\mathrm{ref}}^3\,L} \qquad (16)$$

where:

F: the buoyancy flux, in m^4/s^3
u_{ref}: the wind speed at reference height (normally the building height) in m/s
L: a typical length scale, e.g. the building height or the building width.

The buoyancy flux, F, is defined as:

$$F = g \cdot \frac{(\rho_a - \rho_s)}{\rho_a} \cdot \frac{V_s}{\pi} \qquad (17)$$

where:

g: the gravitational acceleration, in m/s^2

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[30] L_p = 29 was the precise outcome of his calculations. 'L_p > 29' is sometimes referred to as 'Briggs' lift-off criterion'.

V_s: the source volume emission rate, i.e. the volume emission rate of combustion products and entrained nitrogen at their initial (elevated) temperature, in m^3/s
ρ_s: the density of the smoke at elevated temperature, in kg/m^3
ρ_a: the ambient air density, in kg/m^3.

Using:

$$\frac{\rho_s}{\rho_a} = \frac{T_a}{T_s} \qquad (18)$$

and:

$$\Delta T = T_s - T_a = \frac{Q_{conv}}{V_s \cdot \rho_s \cdot c_p} \qquad (19)$$

Equation 17 can be rewritten as:

$$F = g \cdot \frac{(\rho_a - \rho_s)}{\rho_\mathrm{a}} \cdot \frac{V_s}{\pi} = g \cdot \frac{Q_\mathrm{conv}}{\pi \rho_\mathrm{a} c_p T_a} \qquad (20)$$

where:
Q_{conv} the convective heat flux, in W
c_p: the specific heat capacity (at constant pressure) of the plume source, in J/kg·K
T_s: the smoke temperature, in K
T_a: the ambient air temperature, in K.

Equation 20 is an approximation with the following limitations:

- The ratio P_s/P_a (equation 18) is only equal to T_a/T_s for ideal gases and if the average molecular weight of the smoke is equal to that of air. The buoyancy flux will be overestimated if the average molecular weight of the smoke is greater than that of air. If combustion requires oxygen, a substantial amount of nitrogen will be entrained in the smoke. The larger this fraction, the closer the average weight of the smoke will be to that of ambient air.
- The specific heat capacity at constant pressure, c_p, is substance specific and temperature dependent. It is normally assumed that the specific heat capacity of the smoke at elevated temperature is equal to that of air at ambient temperature.
- As can be seen in Table 17, the real specific heat capacity could be substantially different. At elevated temperature, the real heat capacity is larger than that of air at ambient temperature. Ignoring this increase results in an overestimation of the buoyancy flux.

Table 17 Specific heat ratios of air, carbon monoxide, carbon dioxide and water at 25 ºC and 500 ºC (source:[58])

Gas	**Specific heat capacity at 25 ºC and 1 bar (J/kg·K)**	**Specific heat capacity at 500 ºC and 1 bar (J/kg·K)**
Air	1006	1092
Carbon monoxide	1040	1133
Carbon dioxide	846	1158
Water (vapour)	1864	2130

Equation 20 shows that the buoyancy flux *F* is proportional to the convective heat flux Q_{conv}. The proportionality constant is equal to the ratio $g/(\pi\rho_{\mathrm{a}}c_pT_a)$.[31] Different values have been suggested in the literature, e.g. 8.9×10^{-6} by Hall et al. [49], 8.8×10^{-6} by Beychock [57] and 8.56×10^{-6} by Fisher et al. [56].[32] The value 8.8×10^{-6} is typical for air. When assuming an average molecular weight of smoke of 0.03 kg/mol and a specific heat capacity of 1030 J/kg·K[33], the proportionality constant is 8.3×10^{-6}.

Table 18 Proportionality constant for different values of ambient temperature, average molecular weight and specific heat capacity

Molecular weight of smoke	**Ambient smoke density[34]**	**Specific heat capacity**	**Proportionality constant**
0.0289 kg/mol	1.29 kg/m^3	006 J/kg·K	8.8×10^{-6}
0.030 kg/mol	1.34 kg/m^3	030 J/kg·K	8.3×10^{-6}

Further remarks:

- Equation 17 refers to the properties of the emission source. If buoyancy is conserved, equation 17 can also be used for a diluted plume as long as plume volume and plume density are evaluated coherently. The buoyancy of the plume is conserved if p/T is constant. There should be no mass losses (e.g. due to deposition) or energy losses or increases in the plume (e.g. due to evaporation or condensation of water or due to chemical reactions).
- Equation 20 links the buoyancy flux to the convective heat flux, Q_{conv}. This is the convective energy of the undiluted smoke after combustion. Radiated energy and energy lost to the building do not contribute to plume buoyancy and should not be included in Q_{conv}. By using the specific heat capacity at constant pressure, heat losses related to expansion do not have to be considered.
- According to Hanna, Briggs and Chang [59], the dimensionless buoyancy parameter, F/u_{ref}^3L, is roughly equal to 300 L_p if the

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[31] At constant pressure, c_pT_a is constant. The proportionality constant is therefore not sensitive to the choice of ambient temperature. Via the density and heat capacity it does depend on the composition of the gases.

[32] The cited authors expressed Q in MW in their papers and the proportionality constants were 8.9, 8.56 and 8.8, respectively.

[33] The average molecular weight of 0.03 is an average of different fuel compositions tested by RIVM (see Section 3.4.5), assuming that the combustion rate is oxygen-controlled and taking into account the presence of nitrogen in air and smoke. The specific heat capacity of 1030 J/kg·K is used to represent the presence of water vapour in the smoke.

[34] Density at a temperature of 0 ºC and pressure of 1 standard atmosphere (101325 N/m^2).

assumption is used that the atmospheric friction velocity is 10% of the wind velocity.

3.5.5 *Building interactions, buoyancy and dispersion*

The review by Hall and Spanton [53] provides a good summary of the available literature on dispersion modelling for fires in buildings. The report discusses the main characteristics of such fires using a variety of literature sources and outcomes of sets of wind tunnel experiments carried out by David Hall and others between 1980 and 1995. Full details of the various wind tunnel tests carried out by Hall et al. can be found in their research report [49]. Chapter 6 of [50], also by Hall and Spanton, provides little extra information when compared with their earlier review report.

The review report by Ramsdale and Tickle [55] discusses various models for lift-off of ground-based buoyant plumes and puffs. Though the aim of this work was to improve the dispersion modelling for hydrogen fluoride (HF), some sections are also relevant for plume dispersion from fires in buildings. In particular, a useful summary is provided of the early work on buoyant plume dispersion in the 1970s and 1980s, of the wind tunnel experiments by Hall et al. in the 1980s and 1990s, and of a paper by Hanna, Briggs and Chang in response to the latest wind tunnel experiments [59].

Buoyant releases from buildings were extensively investigated by David Hall in at least three series of wind tunnel experiments. These experiments were carried out from the late 1970s to the mid-1990s. The last set of experiments was entirely dedicated to fires in warehouses. The report by Hall et al. [49] discusses the most important findings from all these wind tunnel experiments.

According to [49], the dispersion of smoke plumes cannot properly be described without reference to the way in which the smoke is released from the building and distributed across the building. In other words, earlier attempts to capture smoke dispersion in term of buoyancy and momentum provided an incomplete and inaccurate picture of the dispersion. In particular, if the release was distributed across multiple openings, plume rise was significantly reduced when compared with releases from a single opening or from the shell of a building. At the same time, ground concentrations increased.

According to [53] and [49], the following lessons could be learned from the wind tunnel experiments by Hall et al.:

- If a building structure is largely intact, the heat release will be limited, and the resulting smoke plume is likely to be ground-based (no clear lift-off from the ground). Strongly rising smoke plumes are likely only when there is largely unconstrained ventilation (and a high resultant heat release) due to partial collapse of the building structure.
- There is no clear-cut ‘lift-off’ criterion to discriminate between plumes that either do or do not lift off from the ground. Instead there is a gradual transition.
- For releases with limited buoyancy, the plume can break up into two parts, one part that enters the recirculation zone, mixes,

cools and proceeds as a neutrally-buoyant part, and another part that either bypasses or leaves the recirculation zone with sufficient buoyancy to rise.

- For compact discharges, e.g. from one or a few openings, Briggs's lift-off criterion ($L_p > 29$) is a good indicator of reductions in ground-level concentrations by an order of magnitude or more. For complete clearance of the plume from the ground, the criterion is about an order of magnitude larger.
- As an alternative to Briggs's lift-off criterion ($L_p > 29$), a dimensionless buoyancy flux parameter, F/u_{ref}^3H, can be used, in which F is the buoyancy flux, u_{ref} the wind speed at building height, and H the building height[35] (see Section 3.5.4).
  - For compact releases, ground concentrations start to reduce if the dimensionless buoyancy flux parameter, F/u_{ref}^3H, is larger than 0.02. Reductions of one order of magnitude start to occur when the dimensionless buoyancy flux is around 0.11 (equivalent to $L_p = 29$). For dimensionless buoyancy flux F/u_{ref}^3H above 1, the plume would lift off from the ground almost entirely.
  - If the discharge is distributed across a building, a larger part of the release will be entrained in the recirculation zone behind the building. As a result, plume rise can be greatly reduced and may not be noticeable at all. Ground-level concentrations can be altered by two orders of magnitude if the discharge is distributed rather than compact.
  - Plume lift-off can therefore not be captured in a simple parameter. Instead, the full discharge configuration should be accounted for.
- The effects of wind direction and building shape can alter near field ground-level concentrations by up to an order of magnitude. The lowest ground-level concentrations in the near field occur if the long side of the building is skewed 30° to the wind. In the far field, ground-level concentrations, plume heights and maximum concentrations are largely unaffected by the building shape and its orientation in relation to the wind.

3.5.5.1 Hanna, Briggs and Chang

Responding to the outcomes of the wind tunnel experiments by Hall et al., Hanna, Briggs[36] and Chang [59] proposed a new correlation between ground concentration and buoyancy flux. The proposed correlation combined known physical correlation with fits to data from the wind tunnel tests. According to Hanna, Briggs and Chang, the ground-level concentration could be expressed as:

$$\frac{C(x)\,u\,R^2}{\dot{m}_{tox}} = \frac{e^{-6F^{**0,4}}}{\left\{\frac{1}{3}^3 + 0.03\left(\frac{x}{H}\right)^2 + F^{**2}\left(\frac{x}{H}\right)^4 + \left(\frac{\pi\sigma_y\sigma_z}{R^2}\right)^3\right\}^{(1/3)}} \qquad (21)$$

where F^{**} is the local dimensionless buoyancy flux, defined as:

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[35] In his early work, David Hall used the building height to define the dimensionless buoyancy flux. In his 1995 report, he started using the building width.

[36] Gary Briggs, not to be confused with Brian Briggs, co-author of Atkinson and Briggs [32] (see Section 3.6.4).

$$F^{**} = F_{\mathrm{pl}}/(u_{\mathrm{pl}}{}^{3} W_{\mathrm{pl}}) \qquad (22)$$

and:

$C(x)$: the ground-level centreline concentration as a function of distance x, in kg/m^3

x: the distance from the downwind face of the building, in m

u: the wind speed at building height, in m/s

R: a building scaling length, in m, equal to the minimum of $2H$ and $H^{2/3} \times W^{1/3}$

$\dot{m}_{tox}$: the toxic mass release rate, in kg/s

H: the building height, in m

W: the width of the building perpendicular to the wind, in m

σ_y: the standard deviation of the Gaussian concentration profile in a lateral direction, in m

σ_z: the standard deviation of the Gaussian concentration profile in a vertical direction, in m

F_{pl}: the local[37] buoyancy flux, in m^4/s^3 and equal to $g\ \Delta\rho/\rho_a\ V/\pi$

u_{pl}: the effective wind speed over the depth of the plume, in m/s

W_{pl}: the local lateral plume width, in m.

According to Hanna, Briggs and Chang, equation 21 has at least two elegant features:

- In the absence of buoyancy ($F^{**} = 0$) and for $x = 0$, equation 21 reduces to $CuR^2/\dot{m} = 3$, which is a common expression for the concentration in the recirculation area of the building.
- In the absence of buoyancy ($F^{**} = 0$) and for large downwind distance x, equation 21 reduces to $Cu/\dot{m} = (\pi\sigma_y\sigma_z)^{-1}$, in agreement with the formulation of Gaussian dispersion models.

Equation 21 was developed for releases in which the buoyancy flux was not conserved, in particular HF plumes. Thus, the plume parameters (volume flux, buoyancy flux, effective width and effective wind speed) should be evaluated locally. However, the correlation was fitted against wind tunnel data in which buoyancy was conserved by using fixed values for wind speed and building width.[38] Equation 22 then reduces to $F^{**} = F/u^3W$, which is the common expression for the dimensionless flux. In line with the fit, we will apply equation 21 using fixed values for buoyancy flux, building width (W) and wind speed (u), i.e. $F^{**} = F/u^3W$. This is also how the correlation was presented in the dispersion model review by Hall and Spanton [53].

Hanna, Briggs and Chang also claimed that the ground-level concentration in the event of plume rise is the product of the ground-level concentration in the absence of plume rise and a buoyancy-related correction factor (the 'lift-off term'):[39]

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[37] The volume flux V and the density ρ should be evaluated locally.

[38] The fit of the proposed correlation to the wind tunnel data of Hall et al. is shown in figure 1 in [59]. The three curves in the figure – for downwind distances 60 m, 600 m and 2 km, respectively – can be reproduced using fixed plume width (equal to the building width and independent of downwind distance) and fixed wind speed (also independent of downwind distance).

[39] An important difference between Hanna, Briggs and Chang's correlation (formula 7) and the observations by Hall et al. reported earlier in this section is that Hanna, Briggs and Chang defined the buoyancy flux as F/u^3W, whereas Hall et al. used F/u^3H.

$$C^{buoyant}(x) = C^{neutral}(x) \times e^{-6\cdot(F^{**})^{0.4}} \qquad (23)$$

In their paper, Hanna, Briggs and Chang recognised that equation 23 should be further validated for a wide range of source conditions and meteorological conditions. A comparison with equation 21 shows, however, that equation 23 is valid only if the term $F^{**2}\left(\frac{x}{H}\right)^4$ in the denominator of equation 21 can be neglected, i.e. when $F^{**2}\left(\frac{x}{H}\right)^4 \ll \frac{1^3}{3} + 0.03\left(\frac{x}{H}\right)^2 + \left(\frac{\pi\sigma_y\sigma_z}{R^2}\right)^3$. This condition holds only when the downwind distance (x) is close to zero or when the buoyancy flux is negligible. Given this limitation, equation 23 has little relevance.

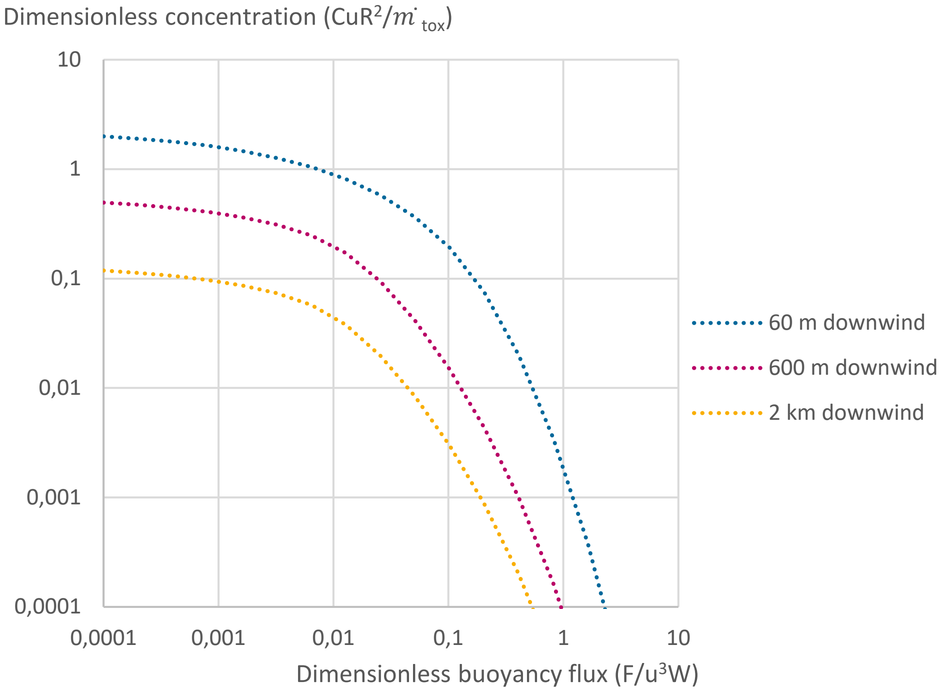

Figure 2 Dimensionless ground-level concentrations using Hanna, Briggs and Chang's correlation for the wind tunnel case (building width 100 m and building height 50 m)

The behaviour of Hanna, Briggs and Chang's correlation (equation 21, hereafter: HBC correlation) is illustrated in Figure 2 for a 100 m wide and 50 m high building (hereafter: the 'wind tunnel case'). The same values were used by Hanna, Briggs and Chang to demonstrate the validity of their correlation (figure 1 in [59]).[40]

- The plot shows dimensionless concentration on the y-axis and dimensionless buoyancy flux on the x-axis. It shows the trend of ground-level concentrations as a function of heat (convective energy) for fixed wind speed, building dimensions and toxic mass

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[40] The figure in this report is identical to figure 1 in [59]. This makes it likely that the building width was used by Hanna, Briggs and Chang to verify their correlation against experimental data, not the local plume width. Building length is not discussed by Hanna, Briggs and Chang. According to [49], the building used in the experiments by Hall et al. (1980) and Hall and Waters (1986) had a width of 100 m, a height of 50 m and a length (or depth) of 50 m.

release rate. Absolute concentration can be obtained by multiplying the dimensionless concentration by $\dot{m}_{tox}/(u \cdot R^2)$.

- As expected, ground-level concentrations reduce with increasing dimensionless buoyancy flux.
- The reduction is about ⅓ if F/u^3W = 0.001 and about ⅔ if F/u^3W = 0.01 (see Table 19).
- A significant drop occurs in the region between 0.01 and 0.1. In this range, the plume behaviour changes from being more or less grounded to largely lifting off.
- The ground-level concentrations continue to drop beyond 0.1 and become negligible beyond 1.

The reduction of ground-level concentrations is slightly larger than David Hall suggested for compact releases in a building wake and much larger than Hall suggested for distributed releases in a building wake.[41] Though the HBC correlation was fitted to data for both compact and distributed releases, it appears to fit compact releases better. This will be an important finding for the remainder of this report.

Table 19 Reduction of ground-level concentrations (relative to zero buoyancy) at different downwind distances, when using the HBC correlation

Dimensionless buoyancy flux	**Reduction at 60 m downwind**	**Reduction at 600 m downwind**	**Reduction at 2 km downwind**
F/u^3W = 0.001	32%	32%	32%
F/u^3W = 0.01	61%	65%	67%
F/u^3W = 0.1	92%	97%	98%
F/u^3W = 1	100%	100%	100%

Figure 3 and Figure 4 show how the absolute concentration of the HBC correlation (equation 21) varies with distance for a 'reference warehouse'.[42] Figure 3 illustrates the effect of wind speed, while Figure 4 demonstrates the effect of increasing combustion rate. The magenta line is identical between the two plots (combustion rate 24 kg/s and wind speed 5 m/s).

The following assumptions were used to generate these graphs:

- warehouse width: 50 m;
- warehouse height: 13.7 m;
- combustion rate per unit area: 0.081 kg/s·m^2;
- convective heat per unit mass combusted: 2 MJ/kg;
- buoyancy flux: $F = 8.5 \cdot Q_{\mathrm{conv}}$[43];
- ratio of toxic release rate to combustion mass rate: 0.34.

Note: These input values are coherent with the inputs used for the reference case described in Chapter 5. The combustion rate is relatively

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[41] According to Hall, ground-level concentrations of compact release in a building wake start to reduce when F/u^3H is about 0.02 (here: F/u^3W = 0.01) and are about 90% reduced when F/u^3H is 0.11 (here: F/u^3W = 0.22). Reductions for distributed releases in a building wake are up to two orders of magnitude smaller.

[42] The 'reference warehouse' will be further discussed in Section 5.1.

[43] Using our own heat balance, we derived $F = 8.3 \cdot Q_{\mathrm{conv}}$ (see Section 3.5.4). $F = 8.5 \cdot Q_{\mathrm{conv}}$ is used to increase consistency with other outcomes presented in this report, in particular those from a method proposed by Atkinson and Briggs; see Section 3.6.4.2.

high and the convective heat per unit mass relatively low. Both values are believed to be conservative.

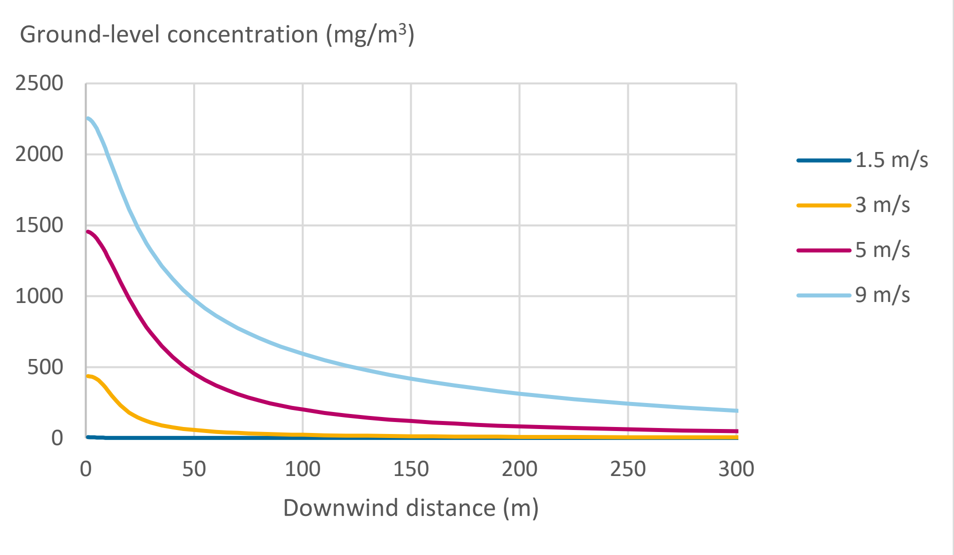

Figure 3 Ground-level concentrations for the reference warehouse (building width 50 m and building height 13.7 m) and combustion rate 24 kg/s

Figure 3 shows that the ground-level concentrations increase with wind speed. This is a result of the reduced plume rise at higher wind speeds. For the lowest wind speed (1.5 m/s) the ground-level concentrations are very close to zero, as the plume almost immediately lifts off from the ground.

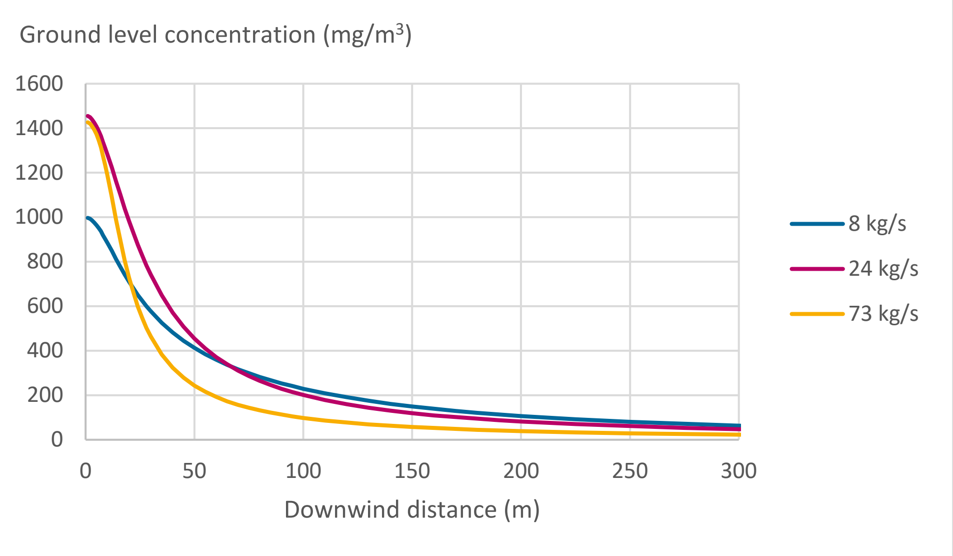

Figure 4 Ground-level concentrations for the reference warehouse (building width 50 m and building height 13.7 m) and wind speed 5 m/s

Figure 4 shows how the ground-level concentration depends on the combustion rate, assuming a fixed wind speed of 5 m/s. The magenta lines in Figure 3 and Figure 4 are identical. The three combustion rates used in Figure 4 correspond to fire sizes of 100 m², 300 m² and 900 m².

The corresponding dimensionless buoyancy fluxes for wind speed 5 m/s are 0.02, 0.07 and 0.2.
The concentrations for 8 kg/s and 24 kg/s in Figure 4 are largely similar. For downwind distances above 50 m, both are higher than those for 73 kg/s. This shows that in the transition zone (F/u^3W between 0.01 and 0.1), the increase in the toxic release rate is balanced by the increase in buoyancy. Beyond 0.1, the effect of increasing buoyancy is stronger than the effect of increasing the toxic mass release rate. Maximum downwind ground-level concentrations are therefore expected to occur with fire sizes with a dimensionless buoyancy flux between 0.01 and 0.1.

3.6 Integral methods

Four methods similar to the Dutch method for calculating the risk of fires in chemical warehouses were found in the literature review and by contacting international colleagues. These four methods, and their differences from the Dutch method, are summarised in the current section.

3.6.1 Flanders

The method used to calculate the risk of warehouse fires causing human fatality in the surrounding area in Flanders, Belgium, is described in chapter 11 of [62]. The method has considerable overlap with the Dutch method [5].

3.6.1.1 Scenarios

In the Flemish method, at least the following effects need to be considered:

- release of toxic combustion products in a warehouse fire;
- release of non-combusted toxic materials in a warehouse fire.

The risk posed by heat radiation from the façade of the building must be considered additionally if the warehouse building does not comply with Flemish fire prevention standards for buildings.

In general, the fire scenarios in the Flemish method are very similar to the ones used in the Dutch method (see Section 2.3). Small differences apply to the fire size distribution to be used for protection levels 2 and 3.

3.6.1.2 Material composition and combustion rate

The derivation of the material composition and the combustion rate are both very similar to the Dutch method. Generic combustion rates per unit area are provided for four types of product:

- general hazardous materials in chemical warehouses: 0.025 $kg/m^2 \cdot s$;
- flammable liquids and pyrophoric substances: 0.1 $kg/m^2 \cdot s$;
- aerosol products in spray cans: 0.3 $kg/m^2 \cdot s$;
- peroxides: 0.5 $kg/m^2 \cdot s$.

3.6.1.3 Source term

Four toxic combustion products need to be considered: nitrogen dioxide (NO_2), hydrogen chloride (HCl), sulphur dioxide (SO_2) and carbon monoxide (CO). The conversion factors are listed in Table 20.

Table 20 Conversion factors for toxic combustion products used in the Flemish method (source: [62])

Conversion	**Conversion factor**
N → NO_2	0.1
H → HCl	1
S → SO_2	1
C → CO	0.05

The survival fractions for non-combusted toxic products are largely similar to those shown in Table 11. Minor differences apply to the survival fractions for automatic hi-ex foam systems using inside air (1.6) and indoor fire attack from in-house firefighters (1.8).

3.6.1.4 Release and dispersion

As in the Dutch method, toxic combustion products and non-combusted toxic products are released into the recirculation zone of the building. After mixing in the recirculation zone, the plume disperses further as a neutrally buoyant plume.

Scenarios and conditions that generate enough plume rise should not be included in the risk calculations. This plume rise criterion is translated into a maximum fire size for consideration in the QRA:

$$A_{max} = \min\left(900, \frac{0.18 \cdot H \cdot u^3}{8.9 \cdot B \cdot H_{eff} \cdot \chi_{conv}}\right) \tag{24}$$

where:

A_{max} the maximum fire size (area) in m^2

H the building height in m

u the wind speed in m/s

B the combustion rate per unit area in $kg/m^2 \cdot s$

H_{eff} the effective combustion energy in MJ/kg (assumed to be 20 MJ/kg)

χ_{conv} the fraction of the combustion energy that is retained as convective heat in the smoke gases (assumed to be 10% on average).

The Flemish lift-off criterion (equation 24) was obtained from the Safety Report Assessment Guidance was published by the HSE in 2002 [63]. In this guidance, the lift-off criterion was presented in the following form:

$$\frac{8.9\, Q_{\mathrm{conv}}}{u^3 H} \geq 0.18 \tag{25}$$

where:

Q_{conv} the convective heat content of the plume in MW

u the wind speed in m/s

H the height of the building in m.

$8.9 \cdot Q_{conv}/u^3H$ is an expression for the dimensionless buoyancy flux, F/u^3L, using the building height as a representative length scale; see Section 3.5.5. For dimensionless buoyancy fluxes above 0.18, plume lift-off is assumed to be significant.

The Flemish criterion (equation 24) is visualised in Figure 5 and applies to a building height of 12.5 m and two different combustion rates per unit area. The combustion energy (20 MJ/kg) and fraction of convective heat (0.1) are defaults. For a wind speed of 3 m/s, the maximum fire size to be considered in the QRA is between 70 and 140 m^2, depending on the combustion rate per unit area. The Flemish cap of 900 m^2 is reached when the wind speed is 5.7 m/s (combustion speed 0.025 kg/m^2s) or 7.1 m/s (combustion speed 0.05 $kg/m^2 \cdot s$).

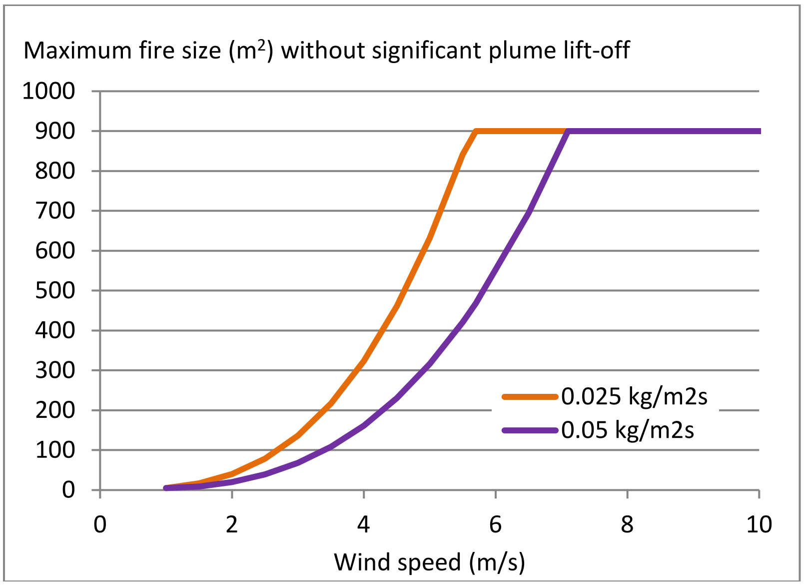

Figure 5 Maximum fire size without plume lift-off for two different combustion rates per unit area (building height 12.5 m)

3.6.2 *Catalonia*

A proposal for a Catalonian risk calculation method was presented in a paper by Seguí et al. [64]. An analysis of historical accidents was carried out to determine common causes and consequences of chemical warehouse fires. Among other factors, the types of substance involved, and their classification, were investigated for 157 warehouse accidents (see figure 3 in [64]). Three 'broadly recognised methodologies' for risk calculation were compared; the 1997 version of the Dutch method, a method published by the US Environmental Protection Agency (EPA) in 2009 and a method published by the UK HSE in 2002 (see also Section 3.6.3). Of these three, the Dutch method was considered to be 'the most scientifically robust and reproducible' method.

Subsequently, the Dutch method was used as a starting point for developing the Catalonian method. Fire scenarios, combustion rate, molecular composition, toxic conversion factors and dose–effect correlations are all identical to the Dutch approach. In contrast to the Dutch approach, however, toxic dispersion is calculated with an Excel tool. According to the authors, this Excel tool is based on a modified Gaussian model from Mannan that takes mixing in the recirculation zone of the building into account. The downwind concentration along the plume centreline is calculated using a relatively simple equation:

$$C(x) = \frac{\dot{m}_{tox}}{(\pi \cdot \sigma_y \cdot \sigma_z + c \cdot A_p) \cdot u} \qquad (26)$$

where:

C(x)	the plume centreline concentration, in g/m^3
x	the downwind distance, in m
m_{tox}	the mass release rate of toxic products, in g/s
σ_y	the horizontal dispersion coefficient, in m
σ_z	the vertical dispersion coefficient, in m
c	a parameter value, equal to 0.2
Ap	the building area perpendicular to the wind, in m^2
u	the wind speed in m/s.

The dispersion coefficients depend on atmospheric stability and distance.

3.6.3 *United Kingdom*

The Safety Report Assessment Guide (SRAG) produced by the HSE [65] provides general guidance on the information that should be included in safety reports for large chemical warehouses.

According to [65], the following types of effects should be accounted for in the risk assessment of chemical warehouses:

- thermal radiation;
- emission of a toxic smoke plume, including unburned toxic material and toxic combustion products;
- explosion;
- run-off of contaminated water.

Explosion risk must be considered in detail only if explosive substances are stored in the warehouse. Deposition of particulate matter and run-off of contaminated water need to be considered to determine the environmental hazard.

The combustion rate should be determined by the operator of the warehouse (or their representative). Table 6 of [65] states that 0.15 kg s^{-1}/m^{-2} is a typical value for the combustion rate, with a margin of 0.1 kg s^{-1}/m^{-2}.

The source term should be determined by the operator of the warehouse. It should include both non-combusted toxic material and toxic combustion products. According to the guidance document, it is almost impossible to calculate the source term reliably. For the survival fraction, 10% is suggested as the default value, with a margin of 5%. HCl, SO_2, HCN, NO_2 and CO are the most important toxic combustion products to be considered for warehouse fires, with proposed conversion factors of 1, 1, 0.05, 0.05 and 0.05, respectively.

For dispersion calculations, the following elements must be taken into consideration:

- The dynamics of the fire: The buoyancy of the plume is relatively low during the early stages of a fire and while a fire is ventilation-controlled. After roof collapse, plume lift-off is likely to occur. Particular attention is required for those stages of the fire where plume rise is limited.

- Wind conditions: Plume rise and plume concentrations at ground level depend on wind speed. The greatest concentrations at ground level are found if the wind speed is high.
- The orientation of the building to the wind: The highest concentrations of toxic substances are found if the long side of the building is perpendicular to the wind and if the release is from the downwind side of the building.

In [65], three general modelling approaches can be identified to calculate dispersion:

1. The use of a 'passive dispersion model with the smoke plume passing through a virtual window not more than a few metres wide or high located at the end of the warehouse'
2. The use of a 'passive dispersion model using a virtual point source at a height above the ground calculated from an assumed plume buoyancy and a maximum plume rise formula similar to those proposed by Briggs'
3. The use of 'a buoyant plume dispersion model based on the work of Ooms or use of a computer program such as ADMS'.

The first approach is considered to be pessimistic. The second approach is deemed acceptable if the assumed height of the virtual source does not exceed about 50 m.

3.6.4 *Atkinson and Briggs*

Graham Atkinson (UK Health and Safety Laboratory, HSL) and Brian Briggs[44] (UK Health and Safety Executive, HSE) published a new method to determine toxic risks from warehouse fires in 2019 [32]. The focus of the method is the health risk of airborne toxic emissions for people who live or work close to the site. Environmental risks are excluded from the scope of the method. Thus, the scope of the method is similar to that of the Dutch method.

The method was designed to be as simple as reasonably possible. Where relevant, a conservative approach was used.

The frequency of serious warehouse fires is assumed to be in the order of 3×10^{-3} per year.

3.6.4.1 Scenarios and source term

The risk assessment uses a fire scenario that represents the early stages of a fire. The duration of this scenario is 30 minutes. It is assumed that people living or working near the warehouse will have the opportunity to escape or be evacuated within this period. Airborne emissions of both non-combusted toxic products (vapours, droplets or particulates) and toxic combustion products need to be considered.

The source term used for non-combusted toxic materials depends on the toxicity of the products involved and of the 'dispersal fraction' (survival fraction). The dispersal fraction depends on storage and fire characteristics and has a value between 0.001 and 0.1. A flow diagram to determine the dispersal fraction for different conditions is provided in

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[44] Not to be confused with Gary Briggs, co-author of Hanna, Briggs and Chang [59].

appendix 1 of [32]. A fairly simple screening test is provided to determine whether a detailed risk assessment should be carried out for the release of non-combusted toxic materials (see module 1 of [32]).

The release of toxic decomposition products (combustion products), must be considered for storage of nitrates, chlorines and substances with high weight-proportions of hetero-atoms (chlorine, sulphur and phosphorus).

- For the storage of nitrates (e.g. ammonium or sodium nitrate), possible decomposition into nitrogen dioxide (NO_2) must be considered. An estimate for the release rate of NO_2 is 20 g/s per tonne of nitrates. This is equivalent to a release of 0.036 kg NO_2 per kg nitrates over 30 minutes. An estimate for the convective heat production is 37 kW per tonne nitrates.
- For storage of chlorines (e.g. swimming pool chemicals, solid hypochlorites, chlorocyanuric acids and salts), possible decomposition into chlorine gas (Cl_2) must be considered. An estimate for the release rate of Cl_2 is 50 g/s per tonne of product. This is equivalent to a release of 0.09 kg Cl_2 per kg product over 30 minutes. An estimate for the convective heat production is 150 kW per tonne of product.
- For storages of substances with high weight-proportions[45] of hetero-atoms (chlorine, sulphur and phosphorus), the generation of HCl, SO_2 and P_4O_{10} must be considered. Some products with hetero-atoms can be excluded from the analysis, as they will not generate significant amounts of HCl, SO_2 or P_4O_{10}. Examples of such products are metal chlorides, metal sulphates and aqueous suspensions (see module 8 in [32]). For the remaining products, it is assumed that all Cl will convert into HCl, that all S will convert into SO_2 and that all P will convert into P_4O_{10}.

For the source term, it needs to be determined how much toxic material will contribute to the fire scenario. The fire scenario represents the early stages of a fire and has a duration of 30 minutes. The total fire duration is expected to be around 3 hours. The toxic amount used for the fire scenario should therefore be between 16.7% and 100% of the total toxic mass in the storage area. A frequency reduction for the scenario is allowed if the amount involved is higher than 16.7% (see module 2 of [32]).

3.6.4.2 Dispersion

The toxic concentration downwind of the building was derived from a series of numerical simulations using the dispersion modelling software ADMS. This computer model has been validated against Hall et al.'s wind tunnel data [66]. The outcomes of the simulations can be used for standard warehouses, i.e. warehouses with planned vent areas in the event of fire in excess of 20 m^2. A different approach must be used for very poorly ventilated warehouses (see module 5 of [32]).

The following assumptions and parameters were used in the numerical simulations:

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[45] High weight proportions: Cl > 25 weight%, S > 25 weight% or P > 5 weight%.

- The smoke is released from the roof of the building with an equivalent release diameter equal to the building width. The wind direction was assumed to be along the long side of the building (see Figure 6). This building orientation was assumed to be conservative for ground-level concentrations downwind of the building.
- Warehouse dimensions: length 75 m, width 25 m and height 10 m.
- The heat produced by the fire ranged between 12.5 MW and 1600 MW.
- The wind speed varied from 2 m/s to 20 m/s.
- The buoyancy number F' (see equation 28) was between 0.002 and 200.

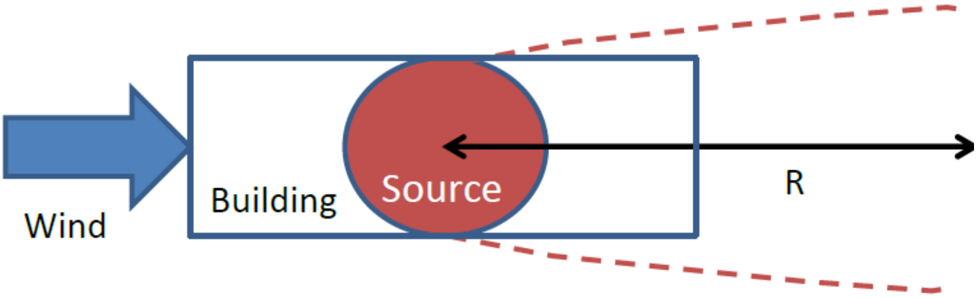

Figure 6 Release geometry used by Atkinson and Briggs for their numerical simulations in ADMS. Figure copied from [32] (with permission).

From these numerical simulations, the following fit was derived for the toxic concentration downwind of the building:

$$C(x) = 0.17 \cdot \frac{\dot{m}_{\text{tox}}}{u\,W^2} \left(\frac{W}{x}\right)^{1.2} \cdot f(F') \qquad (27)$$

where:

$$F' = \frac{26.7 \cdot 10^{-6} \cdot Q_{\text{conv}}}{u^3 W} = \pi \cdot \frac{F}{u^3 W} \qquad (28)$$

$$f(F') = 10^{-\left(0.7 \cdot log_{10} F' + 0.12 \cdot (log_{10} F')^2\right)} \qquad (29)$$

and:

$C(x)$	the ground-level concentration in kg/m^3
x	the downwind distance from the centre of the building, in m
$\dot{m}_{\text{tox}}$	the release rate of toxic products, in kg/s
W	the building width in m
F	the buoyancy flux in m^4/s^3
F'	the buoyancy number (dimensionless)
Q_{conv}	the convective heat flux in W
u	the wind speed in m/s.

The effective heat of combustion is assumed to be 20 MJ/kg. The fraction of energy converted into convective energy is assumed to be 0.5. The convective heat per unit mass is then 10 MJ/kg.

According to Atkinson and Briggs, equation 27 can be applied to buoyancy numbers F' between 0.001 and 4, i.e. dimensionless buoyancy flux between 0.0003 and 1.3.[46]

In their simulations, Atkinson and Briggs assumed that the long side of the building was parallel to the wind direction. While this was demonstrated to yield too conservative outcomes in terms of downwind concentrations (due to more limited mixing in the recirculation zone), it is not the most conservative configuration for buoyancy (due to the more limited mixing in the recirculation zone). Atkinson and Briggs remarked, however, that ‘repeat calculations with the building’s long axis perpendicular to the wind gave fairly similar results (…)’.

Within the recirculation zone of the building ($x \leq 2.5W$), the concentration is assumed to be uniform and equal to the concentration at 2.5 building widths’ distance from the centre of the building: $C(x \leq 2.5W) = C(x=2.5W)$. The width of the plume is assumed to be elliptical. The maximum width of the plume at ground level for a specific concentration of interested is:

$$W_{\max} = 0.75\, {E_{\max}}^{0.75} \tag{30}$$

where $E_{\max}$ is the maximum extent of the plume (in metres) at ground level, i.e. the maximum distance to the concentration of interest along the projected centreline.

The parameter F', referred to as the ‘buoyancy number’ in [32], is the dimensionless buoyancy flux of equation 16 (F/u^3L) of Section 3.5.4 multiplied by a factor π[47], and using the building width W as a typical length scale L. For the sake of coherence with other sections in this report, we will use F/u^3W rather than F' in the remainder of this report.

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[46] Equation 27 actually gives a maximum for $F' = 10^{-0.7/0.24} \approx 0.0012$. The application of equation 27 to buoyancy numbers below 0.0012 (dimensionless buoyancy flux below 0.0004) is therefore physically unrealistic.

[47] According to Atkinson and Briggs, the factor π relates to historic differences in defining the buoyancy flux.

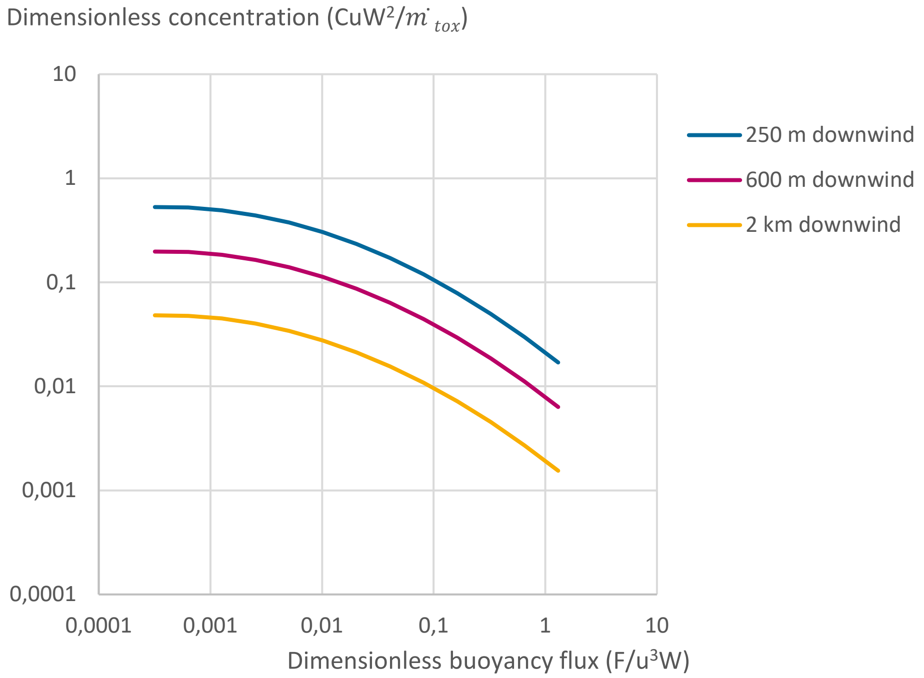

Figure 7 Dimensionless ground-level concentrations using Atkinson and Briggs's correlation for the wind tunnel case (building width 100 m and building height 50 m)

The behaviour of Atkinson and Briggs's correlation (equation 27, hereafter: AB correlation) is illustrated in Figure 7 for a 100 m wide, 50 m long and 50 m high building.[48] In line with the rest of the report, the downwind distance is taken from the downwind face of the building. The dimensionless centreline ground-level concentration reduces gradually with buoyancy flux. In other words, there is no sudden shift from a ground-based plume to a plume that lifts off.

When using the AB correlation, ground-level concentrations are 42% reduced when F/u^3W is 0.01, 80% reduced when F/u^3W is 0.1 and 96% reduced when F/u^3W is 1 (see Table 21). In contrast to the HBC correlation, the effect of buoyancy does not depend on downwind distance. In other words, the relative concentration reduction due to buoyancy is identical between the near field and the far field.

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[48] These are the same input values as were used for Figure 3 (Hanna, Briggs and Chang) but the two graphs cannot be compared directly, as the scaling is different (R^2 versus W^2). In addition, the first reported downwind distance is different – in this case being the distance to the end of the recirculation zone. The reported distances are downwind from the lee side of the building. Distances to the centre of the building (which were used to calculate concentrations) are a half building length longer. Dimensionless buoyancy fluxes below 0.0003 are below the intended scope of application and are not shown in the graph.

Table 21 Reduction of ground-level concentrations[49] when using the AB correlation

Dimensionless buoyancy flux F/u^3W	**Buoyancy number F′**	**Concentration relative to F'=0.001**
0.00032	0.001	1
0.001	0.003	0.96
0.01	0.03	0.58
0.1	0.31	0.20
1	3.14	0.04

Figure 8 and Figure 9 show how the absolute concentration according to the AB correlation varies with distance, using the same inputs as for Figure 3 and Figure 4. The magenta line is identical between the two plots (combustion rate 24 kg/s and wind speed 5 m/s).

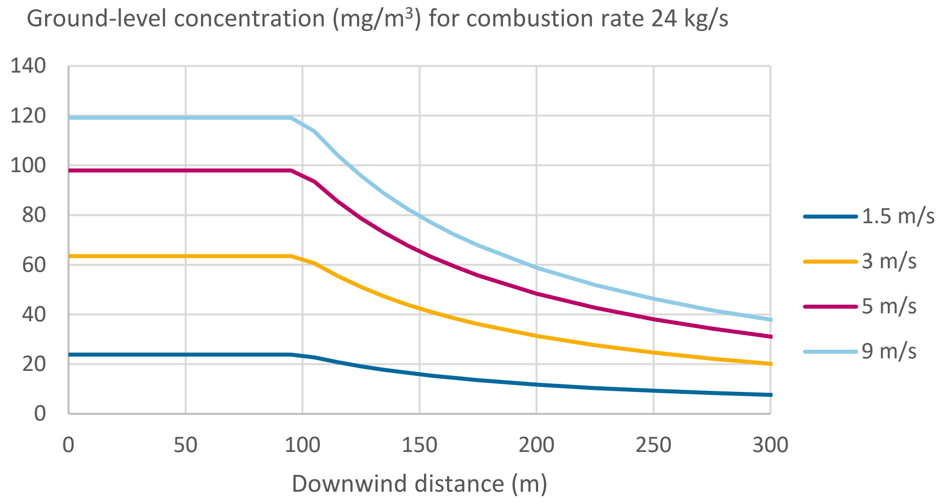

Figure 8 Ground-level concentrations for the reference warehouse (building width 50 m and building height 13.7 m) and combustion rate 24 kg/s

Figure 8 shows that the ground-level concentrations increase with wind speed. This is a result of the reduced plume rise for higher wind speeds. The length of the recirculation zone is assumed to be 2.5 building widths from the centre of the building (2 building widths from the lee side of the building).

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[49] Equation 27 can be applied only to buoyancy numbers (F′) larger than or equal to 0.001. The reductions presented are relative to the ground-level concentrations for F′=0.001. It is assumed that the buoyancy effects will be negligible if F′ is equal to 0.001. The corresponding ground-level concentrations are then equal to those in the absence of any buoyancy.

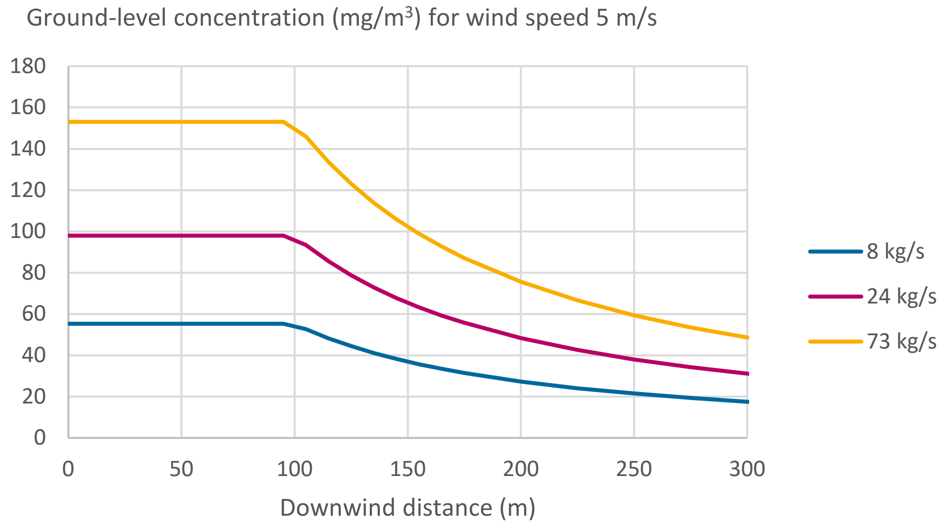

Figure 9 Ground-level concentrations for the reference warehouse (building width 50 m and building height 13.7 m) and wind speed 5 m/s

Figure 9 shows how the ground-level concentration for a wind speed of 5 m/s depends on the combustion rate. Combustion rates differ by factors of 3.[50] The ground-level concentration increases with the combustion rate (or toxic mass release rate), but the increase is not a factor of 3 because there is also an increase in buoyancy, which results in lower concentrations at ground level.

3.6.4.2.1 Identifying the most conservative combustion rate

Increasing the combustion rate implies both increasing the toxic release rate and increasing the buoyancy of the release. Equation 27 can be used to examine which combustion rate would produce the largest downwind ground-level concentrations. The toxic release rate $\dot{m}_{\text{tox}}$ and the buoyancy number *F′* are both proportional to the combustion rate $\dot{m}$.[51]

$$\dot{m}_{\text{tox}} = c_1 \cdot \dot{m} \cdot \frac{u \cdot W^2}{0.17} \qquad (31)$$

$$F' = \frac{\pi \cdot F}{u^3 \cdot W} = c_2 \cdot \dot{m} \qquad (32)$$

where c_1 and c_2 are proportionality constants.

Applying equations 31 and 32 to equation 27 gives:

$$C(\dot{m}) = c_1 \cdot \dot{m} \cdot 10^{-\left(0.7 \cdot log_{10}(c_2 \cdot \dot{m}) + 0.12 \cdot {log_{10}}^2 (c_2 \cdot \dot{m})\right)} \qquad (33)$$

The buoyancy flux that provides the maximum ground-level concentration can be derived by solving $\frac{\partial C}{\partial \dot{m}} = 0$:

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[50] The combustion rates are considered to be representative of fire sizes of 100 m², 300 m² and 900 m², respectively. The corresponding dimensionless buoyancy fluxes for wind speed 5 m/s are 0.02, 0.07 and 0.2.

[51] It is assumed that combustion efficiency does not depend on the combustion rate. This implies that sufficient oxygen is available for combustion.

$$\frac{\partial C}{\partial \dot{m}} = \left(0.3 - 0.24 \cdot log_{10}(c_2 \cdot \dot{m})\right) \cdot 10^{-\left(0.7 \cdot log_{10}(c_2 \cdot \dot{m}) + 0.12 \cdot {log_{10}}^2(c_2 \cdot \dot{m})\right)} = 0 \tag{34}$$

which gives:

$$c_2 \cdot \dot{m} = \frac{\pi \cdot F}{u^3 \cdot W} = 10^{0.3/0.24} = 10^{5/4} \approx 17.8 \tag{35}$$

and:

$$\frac{F}{u^3 W} = \frac{10^{5/4}}{\pi} \approx 5.7 \tag{36}$$

For a fixed wind speed and building width, ground-level concentrations will therefore increase with the combustion rate until the fire has reached the maximum dimensionless buoyancy flux of 5.7.[52]

The combustion rate yielding the largest ground-level concentrations ($\dot{m}_{\text{worst case}}$) can be found by substituting Q_{conv} with $\overline{H_{\text{conv}}} \cdot \dot{m}$:

$$\frac{\pi F}{u^3 \cdot W} = \frac{26.7 \cdot 10^{-6} \cdot Q_{\text{conv}}}{u^3 \cdot W} = \frac{26.7 \cdot 10^{-6} \cdot \overline{H_{\text{conv}}} \cdot \dot{m}}{u^3 \cdot W} \tag{37}$$

where $\overline{H_{\text{conv}}}$ is the average amount of convective energy produced per unit mass (J/kg):

$$\dot{m}_{\text{worst csse}} \approx 17.78 \cdot \frac{u^3 \cdot W}{26.7 \cdot 10^{-6} \cdot \overline{H_{\text{conv}}}} \approx 6.7 \cdot 10^5 \frac{u^3 \cdot W}{\overline{H_{\text{conv}}}} \tag{38}$$

3.7 Computer models

Numerous models have been developed to model the development of fires in buildings. These models normally model the initial fire development within a room or compartment and the subsequent spreading of the fire to adjacent rooms or compartments. The models generally calculate fire intensity, flame height, temperatures at various heights and mass flow rates over time. They require simplified assumptions about the type of materials in the enclosure, their combustion characteristics, the storage conditions, the availability of oxygen, etc. Though these models are detailed in terms of available outputs, they are quite simplistic in terms of inputs and use of physics. As a result, their overall accuracy is questionable. More information on these enclosure fire models can be found in [35].

Few, if any, readily available models exist that combine fire development calculations with smoke plume dispersion calculations. To cite the review of smoke plume models commissioned by the UK ADMLC [53]:

'There is no standard software or methodology generally available for dealing with smoke plumes (some exist, but are not publicly available) and, as a result, the application of different models and methods is largely ad-hoc. Some calculations use conventional dispersion models with little

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[52] The ground-level concentration corresponding to this worst-case buoyancy flux is 8.3‰ of the ground-level concentration in the absence of buoyancy (buoyancy number 0.001).

reference to specific smoke plume properties. In general, these conventional models do not account very well for smoke plume behaviour, though some attempts have been made to adapt them. The application of the limited variety of simple smoke plume models and empirical rules is not standardised. Similarly (with one exception), there is no organised archive of the existing limited experimental database that can be used for common validation purposes. Nor are there any agreed standard test cases for smoke plume modelling intercomparison, which should include specific conditions known to affect smoke plume behaviour.'

A similar remark is made by Purser [46]:

'The limitations of all modelling methods are that, although some aspects of fires, especially air entrainment and smoke movement within and from building enclosures, can be calculated with reasonable accuracy, the predicted conditions, especially in terms of the time-concentration curves for toxic products, are heavily dependent upon a range of input assumptions. Existing models are not fully capable of simulating the complexities of the actual fire source term (the processes whereby a fuel is pyrolised and then combusted), and while for a given fire they can predict the yields of 'major species' such as CO_2 with reasonable accuracy, the prediction of 'minor species', which include essentially all the products of interest to toxicologists, is much less certain.'

In the UK, the software program FIREPEST was developed to assess risks from emissions of toxic products from fires in chemical warehouses. This model was developed by the HSL in the late 1990s on behalf of the HSE. The development of a fire and the source term could be calculated by defining the fuel and storage characteristics. Outcomes of wind tunnel experiments by David Hall were used to determine downwind concentrations. The latest update of the software (FIREPEST III) was carried out in 1998. Currently, the model is no longer in use.

More recently, the HSL has used the commercial software tool ADMS to calculate the dispersion of emissions of toxic products from building fires [32]. According to a paper by Carruthers et al. [66], this program can indeed be used for that purpose. To our knowledge, the program cannot be used to calculate fire development or individual risk.

Boot and Pérez reported in 2020 that the software program EFFECTS now contains a plume rise model for warehouse fires and pool fires [67]. The formulae that are used to calculate plume rise were derived for pool fires in open air. Building effects are not considered in the model. Nevertheless, according to Boot and Pérez, the predicted ground-level concentrations show reasonable agreement with ground-level concentrations observed by David Hall et al..

4 Weaknesses in the current method and possible improvements

4.1 Introduction

In the previous chapter, a literature review was carried out to investigate various components of the Dutch calculation method for chemical warehouse fire risks. These results are used in the current chapter to identify weaknesses in the current Dutch approach and to provide recommendations for improving that method.

For any weakness, three types of solution are possible:

- Substitution: replacing a single element by another element, e.g. a parameter value by another value. This solution can be applied if the set-up of the model is good but when specific choices of parameter values can be improved.
- Increasing the level of detail: making further distinctions between different situations, thereby increasing the level of detail and complexity of the method. This solution can be applied if the current method is too simple and if reliable data are available to increase the level of detail. The required warehouse and storage properties should be known, as well of the effect of these properties on fire hazard and risk. In addition, increasing the level of detail is desirable only if it has a significant impact on the outcomes of the consequence or risk calculations. Insignificant changes are not worth the time and effort required to make the change.
- Reducing the level of detail: simplifying elements of the model that cannot be fully justified. This may involve reducing the number of parameters required for a calculation or removing distinctions in the method that lack scientific underpinning. Influences and effects that are highly uncertain should not be used in the method.

It became apparent from the literature review that a lot of uncertainties apply when assessing the risk of toxic health effects from chemical warehouse fires. To name a few:

- The products stored in warehouses vary with time and it is difficult to obtain storage data that are representative over time.
- Fire spread and fire intensity depend on the types of packaging used, the stack height and the availability of oxygen. These variables may change in time, may vary between different parts of the fire compartment and may change during the cause of the fire.
- Automatic fire suppression systems can limit fire growth but may not be activated or fail in their response. The actual response of the fire suppression system is unknown prior to the fire.
- Production rates for toxic components depend on combustion efficiency, which depends on the fire intensity and the availability of oxygen. They will vary during the cause of the fire and are difficult to predict with great accuracy.

- Emissions from the building depend on the size, number and location of openings in the building. The emissions will also vary during the cause of the fire and are also difficult to predict with great accuracy.
- Subsequent dispersion depends on the wind speed, the interaction of the building with the wind and the convective energy that is conserved in the plume. The number of possible variations is large.

In the light of these uncertainties, it is deemed impossible to calculate risks and effects with great accuracy. Calculation methods can therefore provide only rough estimates of the off-site risks and of the distances where significant health effects are expected.
In the following subsections, the different elements of the risk assessment are discussed. Each subsection ends with an outline of areas where the existing Dutch risk calculation method might be improved.

4.2 Warehouse fire frequency

4.2.1 Considerations

Warehouse fire frequencies were not studied in detail in this report. In the current method, the assumed frequency of a warehouse fire that reaches a size of at least 20 m^2 is 8.8×10^{-4} per compartment per year. Two references were found in which the proposed warehouse fire frequency was substantially higher than this value (see Section 3.2).

- According to a study by WS Atkins Consultants in 2003 [31], the likelihood of a fire that will not self-extinguish or will not be immediately extinguished by people nearby is in the order of 10^{-2} per year per unit or between 1×10^{-5} and 3×10^{-5} per m^2 floor area per year.
- In a study by the HSE [19], the likelihood of a serious fire in a chemical warehouse (causing widespread structural damage to the roof) was assumed to be in the order of 3×10^{-3} per year.

4.2.2 Recommendations

The warehouse fire frequency is required for the risk calculation. Despite unsuccessful attempts in the past, it is assumed that sufficient data are now available to determine warehouse fire frequencies more accurately. It is therefore recommended that the warehouse fire frequency figures be updated.

4.3 Fire development

4.3.1 Considerations

Fire development is expressed in terms of a set of fire scenarios. Each scenario consists of a fire size, a ventilation rate and a duration (see Section 2.3). The sizes, ventilation rates and durations to be used, and their relative probabilities, depend on the protection level of the fire compartment. For protection level 1, a further distinction is made between various types of automatic fire suppression system.

The underpinning of the fire scenarios and their relative probabilities is weak. A brief survey was used to determine fire sizes and relative probabilities for a warehouse with an automatic sprinkler system. Different groups of experts then adapted these outcomes to other fire suppression systems. Additional assumptions were made when the maximum fire size was increased from 300 m^2 to the full size of the storage area in 1997.

In reality, fire growth depends on many parameters. These include the size of the fire compartment, the types of materials that are stored and their packaging, the storage height, separation distances between stacks and racks, building height, the ventilation rate in the building and the presence of open doors, windows or roof vents. The effect of automatic fire suppression systems depends on the time of activation of the system (if activated at all) and the quality of the response.

Several studies were found that provided estimates for the likelihood of a successful response of automatic fire suppression systems. These were discussed in Section 3.4.7. These estimates showed scatter and the applicability of various data to Dutch chemical warehouses remains unknown. No specific database exists from which the likelihood of successful suppression of fires in Dutch chemical warehouses can be extracted.

For most automatic fire suppression systems, the current Dutch calculation method identifies five different fire sizes: 20 m^2, 50 m^2, 100 m^2, 300 m^2 and 900 m^2. This level of detail is high in comparison with the uncertainties in their effect mentioned above. In Section 3.3.11, it was proposed to distinguish only three scenarios: successful fire suppression, failure and partial failure:

- Fully effective: The fire is either extinguished or kept within designed safe limits.
- Failure: The suppression system does not perform as intended and the fire is not controlled. As a result, the fire size increases and eventually flashover will occur. The suppression system may, however, delay the fire growth and the time until flashover occurs.
- Partial failure: The suppression system does not perform as intended but does succeed in restraining fire growth and preventing flashover.

In the most recent version of the technical standard for PGS15-warehouses [10], it was made explicit that the local fire brigade will not try to extinguish a fire in a compartment if the fire compartment does not contain an automatic fire suppression system. Instead, they will try to prevent the fire from spreading to other compartments or buildings. Therefore, the fire will eventually consume the entire fire compartment.

A last point of interest is that a recent (2016) ruling allows both general trade goods and hazardous substances to be stored in the same fire compartment. A reviewer of this report expressed concerns about Li-ion batteries, which can now be stored in the same fire compartment as combustible products. A significant amount of heat can be released when Li-ion batteries catch fire. In addition, hydrogen fluoride (HF) can be released.

Recommendations
The development of a fire is complex and depends on many parameters. Considering the large number of variables and uncertainties, it is

impossible to assess fire growth with great accuracy. The level of detail in the current method, in terms of the number of fire scenarios used, is high. It is therefore recommended to simplify this part of the method as follows:

- Negligible fire size in case of fully successful automatic fire suppression. No off-site risk calculations are required for fully successful automatic fire suppression.
- Fire size equal to the size of a storage section for partially successful automatic fire suppression.[53]
- Fire size equal to the full floor area for largely or completely failing automatic fire suppression and in the absence of automatic fire suppression systems.

It should be further investigated whether the proposed fire sizes are indeed representative of partially successful and failing automatic fire suppression.

The maximum fire size to be used should depend on the way in which the buoyancy of the release is accounted for (see Sections 4.5 and 5.3). One of the options is to consider only scenarios with a buoyancy flux below a critical value. If this option is used, the maximum fire size to be used in the risk calculation will be further restricted.

4.4 Combustion rate

4.4.1 Considerations

In the current method, the combustion rate is the minimum of the fuel-restricted combustion rate and the oxygen-restricted combustion rate. This is physically realistic. However, the assumptions for calculating the fuel- and oxygen-restricted combustion rates are too simplistic:

- The fuel-restricted combustion rate currently depends only on the fraction of flammable liquids (ADR class 3) in the fire compartment. In reality, the combustion rate also depends on the height of stacks and racks in the storage, the fraction of flammable solids (ADR class 4) and the fraction of oxidising substances (ADR class 5). The storage height is particularly important for ASRSs. Taking into account these new factors will probably increase the predicted combustion rate per unit area.
- The oxygen-restricted combustion rate currently depends on the building volume and the building ventilation. A ventilation rate of 4 building volumes per hour is assumed when doors are closed and an infinite ventilation rate is assumed when doors are open. This approach is a simplification of reality. On the one hand, open doors do not provide an infinite amount of air. On the other hand, the effects of air intake through open windows and roof vents are currently not accounted for. More detailed methods are available to calculate the mass of air flowing into a building as a function of the indoor temperature and the size and height of doors, windows and roof vents (see Section 3.3.4). Determining the temperature to be used in these calculations may be difficult.

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[53] The Dutch technical standard for storage of packaged hazardous goods in warehouses [10] requires that the size of the storage section should not exceed 300 m^2. If multiple sections have different sizes (<300 m^2), the size of the largest storage section can be used as a conservative approach.

It will also be a challenge to identify the likelihood of doors, windows and roof vents being open.

In the previous subsection, it was recommended that the number of fire sizes that must be considered in the risk calculation be reduced. It can also be decided to no longer distinguish between fuel-restricted and oxygen-restricted combustion rates. For a given fire size, the fuel-restricted combustion rate is always greater than the oxygen-restricted combustion rate. A conservative simplification would be to only use the fuel-restricted combustion rate. If so, the likelihoods of open doors, windows and roof vents do not need to be considered.

Lastly, the maximum fire size to be used in the risk calculation should depend on the way in which the buoyancy of the release is accounted for (see Sections 4.5 and 5.3). One of the options is to only consider scenarios with a buoyancy flux below a critical value. If this option is used, the combustion rate per unit area, whether fuel-restricted or oxygen-restricted, becomes irrelevant for the largest scenario to be considered.[54]

4.4.2 Recommendations

The current method distinguishes between fuel- and oxygen-restricted combustion rates. Simplifications are used to calculate these combustion rates. Therefore, the current method gives a false sense of precision. Adding detail will be time-consuming and may not result in higher precision if the required input parameters are uncertain. It is therefore recommended to investigate whether the method can be simplified by taking into account only the fuel-restricted combustion rate. This is a conservative approach.

The following actions are recommended:

- Investigate whether it is feasible *not* to consider the amount of oxygen supplied to the fuel and to assume that the combustion rate is always fuel-restricted. This is a conservative approach that increases the simplicity of the method.
- Investigate whether the fraction of flammable solids (ADR class 4) and of oxidising substances (ADR class 5) can be significant in warehouses.
- If so, identify the fuel-restricted combustion rates for these types of substances.
- Investigate the fuel-restricted combustion rate for high-rack storage.

4.5 Effects of buildings and buoyancy on ground-level concentrations

4.5.1 Considerations

In the Dutch method, the smoke that is released from the building will mix in the recirculation zone of the building and then disperse neutrally, i.e. with a constant plume centreline height away from the building wake. From expectations about the progress of a fire in a fire compartment, a maximum fire size of 900 m^2 was implemented in the

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[54] In this option, the maximum fire size is inversely proportional to the combustion rate per unit area (the higher the combustion rate per unit area, the lower the maximum fire size). The toxic release rate, on the other hand, is proportional to the combustion rate per unit area and the fire size. Thus, the worst-case toxic release rate will be independent of the combustion rate per unit area.

current calculation method (see Section 2.3.3.4). This maximum fire size applies to all weather classes. No assessment of buoyancy effects was carried out when defining the maximum fire size. The literature study showed, however, that buoyancy is important and should be accounted for when calculating ground-level concentrations.

In the literature, several approaches were found in which the effect of plume rise was either fully present (on) or absent (off), depending on a critical value for buoyancy. An example is the Flemish criterion $F/u^3H < 0.18$ [62], which was earlier published by the HSE [36]. These approaches neglect the fact that plume rise is a gradual process rather than a sudden event, in particular when combined with building effects (e.g. [53], [55]). At the same time, these approaches are simple to use and may not perform worse than more complex approaches.

Publications by Hall and others [53], [49] showed that ground-level concentrations are reduced by one order of magnitude when the dimensionless buoyancy flux F/u_3H is around 0.11 and the release is compact. For F/u_3H larger than 1, the plume will lift off from the ground almost entirely. For distributed releases from buildings, the effect of buoyancy is much smaller, and downwind ground-level concentrations can be two orders of magnitude higher than with compact releases [53], [49].

Hanna, Briggs and Chang [59] provided a correlation between the ground-level concentration, release rate, building width, buoyancy flux and downwind distance (equation 21; HBC correlation). The correlation combined physical arguments with fits to experimental data from Hall et al. [49]. When using this equation, ground-level concentrations reduce noticeably if the dimensionless buoyancy flux F/u^3H is 0.01 and become negligible when this exceeds 1.[55] This behaviour is largely in line with Hall’s observations for compact releases.

Atkinson and Briggs [32] came up with an alternative correlation between ground-level concentration, release rate, building width, buoyancy flux and downwind distance (equation 27; AB correlation). This correlation was a fit of numerical simulations with the computer code ADMS. In these simulations, the smoke was assumed to be released from the roof of the building with an equivalent release diameter equal to the building width. It is therefore representative of distributed releases.

The differences between the two correlations are illustrated in the following graphs.

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[55] See Table 19. In this ‘wind tunnel case’, the building width (W) is twice the building height (H). As a result $F/u^3W = ½ \cdot F/u^3H$.

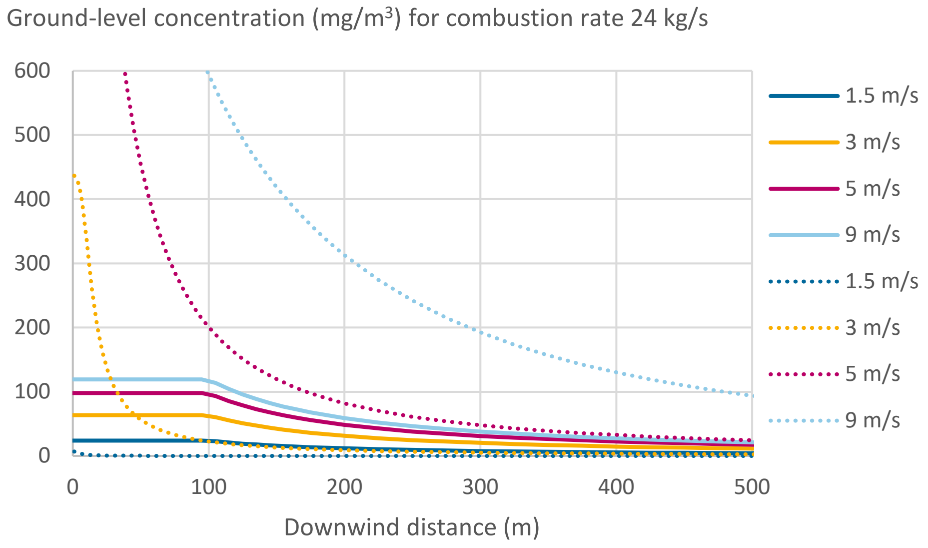

Figure 10 Ground-level concentrations according to the AB correlation (solid lines) and HBC correlation (dotted lines) for the reference warehouse (building width 50 m and building height 13.7 m) and combustion rate 24 kg/s

Figure 10 shows predicted ground-level concentrations for the reference warehouse, assuming a fixed combustion rate of 24 kg/s. The corresponding toxic mass release rate is 8.2 kg/s, the heat release rate 49 MW. The corresponding dimensionless buoyancy fluxes are 2.5 for wind speed 1.5 m/s, 0.3 for 3 m/s, 0.07 for 5 m/s and 0.01 for 9 m/s. See also Section 3.5.5.1.

- One reason for the difference between the two correlations is the different approach for calculating the ground-level concentration in the recirculation zone (up to 100 m downwind from the side of the building, according to Atkinson and Briggs). The AB correlation assumes a constant concentration in the recirculation zone. The HBC correlation does not provide such a constant concentration in the recirculation zone. Within the recirculation zone, the outcomes for AB are typically lower than those for HBC.
    - Atkinson and Briggs assume a release from the roof of the building with an equivalent release diameter equal to the building width. The fraction of the release that is entrained into the recirculation zone will fully mix in the recirculation zone. The resulting concentrations are relatively low.
    - Hanna, Briggs and Chang have fitted outcomes of wind-tunnel experiments. Apparently, concentrations were not uniformly mixed in the recirculation zone in many tests, resulting in relatively large concentrations.
- A second difference is the decay in concentrations with downwind distance. This decay is much stronger for the HBC correlation than for the AB correlation. In the HBC correlation, the reduction due to buoyancy increases with distance. The plumes lift off, and continue lifting off, resulting in larger reductions of ground-level concentrations with increasing distance. Atkinson and Briggs propose a fixed reduction factor due to buoyancy, independent of downwind distance.

Figure 11 shows the dimensionless concentrations for three downwind distances using the wind tunnel case (building width 100 m and building height 50 m). These are the values that were used by Hanna, Briggs and Chang in their paper to validate the wind tunnel experiments of David Hall. The first downwind distance in the graph represents the end of the recirculation zone in Atkinson and Briggs' approach and the other two distances are further downwind.[56] Both correlations have been scaled using dimensionless concentration $CuW^2/\dot{m}_{tox}$, with C the downwind ground-level centreline concentration, *u* the wind speed, *W* the building width[57] and $\dot{m}_{tox}$ the toxic mass release rate.

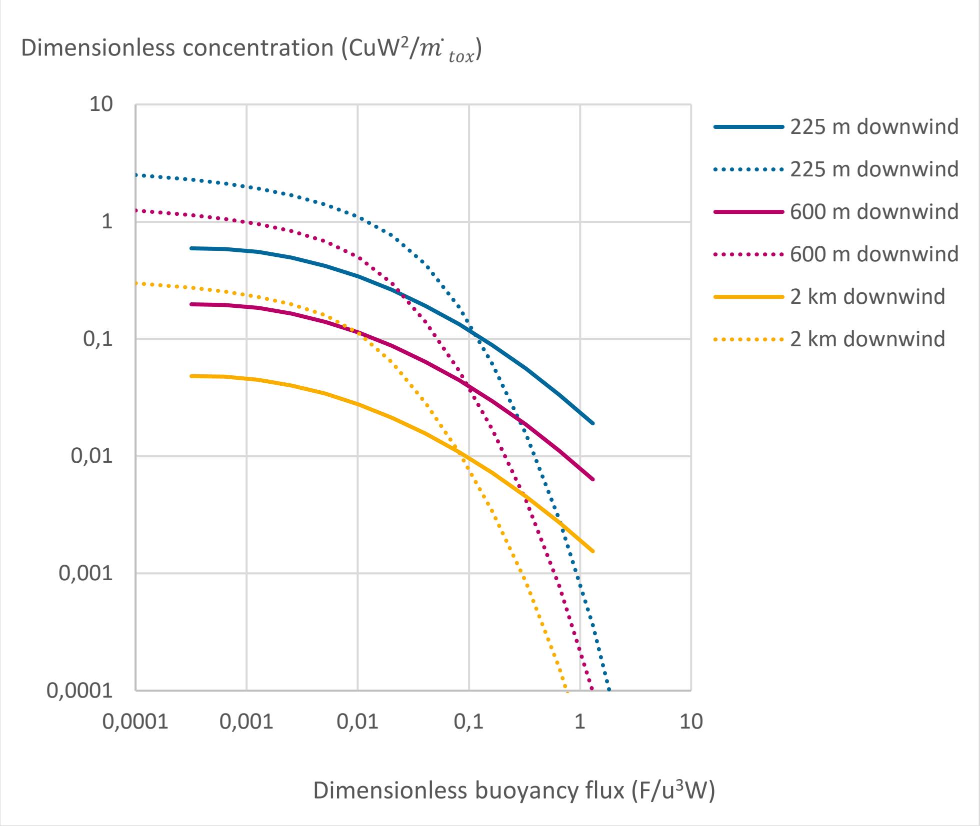

Figure 11 Dimensionless concentrations according to the AB correlation (solid lines) and the HBC correlation (dotted lines) for the wind tunnel case (building width 100 m, building length 50 m and building height 50 m)

The following observations can be made from Figure 11:

- For dimensionless buoyancy flux F/u^3W below 0.01, the concentrations using the HBC correlation (dotted lines) are a factor of 4–6 higher than those predicted by the AB correlation (solid lines).
- The lines cross when the dimensionless buoyancy flux is around 0.1.[58] Beyond this value, the AB correlation gives higher dimensionless ground-level concentrations.

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[56] According to Atkinson and Briggs, the recirculation zone is 2.5 building widths (250 m) long, measured from the centre of the building. The distance from the centre of the building to the side of the building is half the building length (25 m).

[57] In their paper, Hanna, Briggs and Chang used R^2 instead of W^2 to make the concentrations dimensionless.

[58] The exact value depends on the downwind distance. The value is specific to the warehouse configuration considered.

- For dimensionless fluxes beyond 0.01, the dimensionless concentrations reduce faster with dimensionless buoyancy flux when using the HBC correlation (dotted lines). The behaviour of the HBC correlation is consistent with Hall's wind tunnel outcomes for compact releases (see Section 3.5.5.1). The AB correlation is derived from model runs for distributed releases.
- From dimensionless buoyancy fluxes of 1 and above, the AB correlation gives ground-level concentrations that are more than one order of magnitude higher than those of the HBC correlation.

Overall, the differences between the two correlations can be summarised as follows:

- The HBC correlation tends to produce higher ground-level concentrations near the building. This correlation appears to have less mixing in the recirculation zone of the building. This is coherent with the idea that this correlation better fits compact releases, while the AB correlation applies to distributed releases.
- The effect of buoyancy is stronger in the HBC correlation. With increasing buoyancy, ground-level concentrations reduce faster than with the AB correlation. This is also coherent with the idea that the HBC correlation applies to compact releases, while the AB correlation applies to distributed releases.
- The effect of buoyancy increases with distance when using the HBC correlation and not when using the AB correlation. This element of the HBC correlation is expected to be more realistic.
- Which correlation gives the larger ground-level concentration depends on building geometry, buoyancy (convective heat) and distance.
- Wind tunnel experiments have illustrated that ground-level concentrations depend on many parameters. Together, the two correlations are expected to define the range of possible outcomes.

4.5.2 *Recommendations*

In the current method, the plume is assumed to remain grounded for fire sizes up to 900 m^2, irrespective of wind speed. This approach is too simple, as reductions of ground-level concentrations can be significant if the wind speed is limited. For high wind speeds, on the other hand, buoyancy effects can be small even if the fire size is larger than 900 m^2.

The papers by Hanna, Briggs and Chang [59] and by Atkinson and Briggs [32] can be used to identify which ground-level concentrations are deemed realistic for a specific scenario. Both papers were directly or indirectly based on David Hall's wind tunnel experiments [49]. Between the two, the predicted concentrations can differ by roughly a factor of 5. This difference is assumed to reflect the complexity of the topic in general, and differences between compact releases and distributed releases in particular. Together, the two correlations define the range of possible outcomes.

The following options for improving the Dutch method with respect to buoyant behaviour of the plume should be further explored.

1. Improve the dispersion model in order to account for gradual lift-off of the smoke plume. Ideally, the dispersion model should

combine aspects of mixing in the recirculation zone and lift-off due to buoyancy. For SAFETI-NL, this requires a modification of the model code. No readily available model was found in the literature. Two correlations were found that were specifically proposed for fires in buildings. One is more suited for compact releases, while the other is more suited for distributed releases. Depending on the scenario and the location, either of the two could result in larger/smaller predicted concentrations.

2. Test whether acceptable concentration outcomes can be obtained with the current version of SAFETI-NL by modifying some of the parameters to be used for the consequence and risk calculation.

The effect of possible modifications to the Dutch risk calculation method could be compared with the concentrations predicted by the HBC and AB correlations (which together span the range of outcomes).

The following three approaches[59] can be tested:

a. Mimic plume rise using an elevated release temperature. This option requires deselecting the building wake model in SAFETI-NL (as the building wake model suppresses lift-off). The main challenge will be not to overpredict buoyancy in the absence of any mixing in the recirculation zone.
b. Modify the source term in order to correct for buoyancy. Plume rise results in reduced ground-level concentrations. If this reduction can be calculated in a fairly simple way, the source term to be used as input for dispersion calculations can be modified as a workaround. Being a workaround, this is not the preferred option. However, it can be a solution if the other options fail.
c. Use a better underpinned criterion for maximum fire size in the risk calculation method. This is for example the approach used in Flanders. The new criterion should consider both wind speed and building characteristics. This approach is fairly simple and ignores the fact that lift-off is a gradual process, not a step change. In addition, it does not capture the difference between compact and distributed releases. However, simplicity can also be an advantage and is acceptable if the resulting consequence and effect distances remain within acceptable limits.

These options are further explored in Section 5.2 of this report.

4.6 Scenario duration

4.6.1 Considerations

For fire sizes up to 100 m^2, the scenario duration is supposed to be equal to the time required to extinguish the fire, with a maximum of 30 minutes. For fire sizes of 300 m^2 and 900 m^2, the scenario duration is 30 minutes. This value is identical to the maximum release duration for releases from storage and process installations at Seveso sites [2]. It is further assumed that building collapse within 30 minutes is unlikely. The maximum duration appears to be of the right order of magnitude. The same values are also used elsewhere (e.g. [62] and [32]).

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[59] Including Option 1, there are four options in total.

4.6.2 Recommendations

None.

4.7 Combustion products and conversion factors

4.7.1 Considerations

The current method considers only three toxic combustion products: nitrogen dioxide, sulphur dioxide and hydrogen chloride. Carbon monoxide (CO) is currently not considered but could be produced in relevant quantities. The method used in Flanders [62] and the method proposed by Atkinson and Briggs [32] also require inclusion of the toxic effects from CO in the risk assessment. Both use 5% as the value to be used for the conversion of carbon into CO.

Since 2016, both general trade goods and hazardous substances can be stored in the same fire compartment. A reviewer of this report expressed specific concerns about Li-ion batteries being stored in the same fire compartment as classified hazardous substances. A significant amount of heat can be released when Li-ion batteries catch fire. In addition, hydrogen fluoride (HF) can be released.

4.7.2 Recommendations

- Take the risk of dispersion of CO into consideration, using a conversion factor of 0.05. This will result in a higher mass release rate. The increase depends on the assumed composition of the materials that are stored in the warehouse.[60]
- Identify when the release of HF from Li-ion batteries is significant compared with the release of toxic combustion products and non-combusted toxic products.

4.8 Effects of exposure to toxic substances

4.8.1 Considerations

Dosis-effect relations are used to translate toxic exposure to a probability of fatality. The underlying probit values for specific toxic substances were derived in the 1990s [17]. New probit values with a better scientific underpinning have been proposed in recent years [18]. Their use in risk calculations has not yet been approved by the relevant Ministry.

For mixtures of toxic substances, the source term is equal to the sum of the source terms for the different toxic components in the mixture.

- The calculated risk depends on the expected likelihood of fatality for exposure to the toxic mixture. Survival rates are first calculated per component and are subsequently multiplied as if they are independent of each other. This independence is not deemed realistic.
- The effect contour involves the area where the lowest 'life-threatening value' of any of the toxic products is exceeded. This approach can be very conservative if the fraction of this 'most toxic' component in the mixture is small.

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[60] For the reference case that is investigated in Chapter 5, the mass rate for CO is about 10% of the summed mass rates for NO_2, SO_2 and HCl (see Table 28). For this case, an average material composition with significant amounts of N, S and Cl was assumed. For lower amounts of N, S and Cl, the mass fraction of CO will be higher.

These issues apply not only to warehouses, but to all types of activities for which off-site risks are calculated [5].

4.8.2 *Recommendations*

It is recommended to use the recently derived probit values as these have a better scientific underpinning than the ones that are currently used. For exposure to a mixture of toxic substances, it is recommended to improve the method for calculating the likelihood of fatality and the method for identifying the representative life-threatening concentration.

5 Accounting for building and buoyancy effects

In Chapter 4, several options for improving the existing Dutch method were suggested. One of these was to better account for the effect of buildings and buoyancy. Several options for improving the modelling were discussed in Section 4.5. These options are further investigated in this chapter.

A reference case is used to illustrate the workings of the current method. This case was obtained from a Dutch user of SAFETI-NL. According to this user, this case results in excessively large consequence areas when the current Dutch method is used.

The reference case and the outcomes using the current method are described in Section 5.1. When comparing these outcomes with the literature (Section 5.1.2), it becomes clear that the effect distances of the current Dutch method are too large. Several options to better account for buoyancy and lift-off of the plume are discussed in Section 5.2. A summary of the investigation is provided in Section 5.3.

5.1 Reference chemical warehouse

For the purpose of testing the validity of the current method and of possible improvements to it, the following reference PGS15-warehouse was obtained from a user:

- warehouse storage area: 2500 m^2;
- building length: 50 m;
- building width: 50 m;
- building height: 13.7 m;
- fire suppression system: automatic hi-ex foam system with outside air;
- average material composition of stored products: $C_{3,9}H_{8,5}O_{1,06}N_{1,17}S_{0,51}Cl_{0,46}P_{1,35}R_x$.[61] Average molecular weight of stored products: 163 g/mol. Mass fraction of nitrogen: 0.1. Mass fraction of chlorine: 0.1. Mass fraction of sulphur: 0.1;
- mass fraction ADR class 3 flammable liquids in the storage: 0.75.

The building size, the mass fractions of nitrogen, chlorine and sulphur and the mass fraction of flammable liquids in this reference case are all conservative.

5.1.1 Results when using the existing Dutch method

For an automatic hi-ex foam system with outside air, five fire sizes should be considered in the risk calculation: 20 m^2, 50 m^2, 100 m^2, 300 m^2 and 900 m^2 (see Table 1). As the suppression system uses outside air, it is assumed that the combustion rate will not be limited by oxygen supply. Therefore, only scenarios for fuel-controlled combustion need to be considered. These are shown in Table 22. The total relevant fire frequency is 8.8×10^{-4} per year. The likelihood of a fire size of 100 m^2 or more is 2% of the total fire frequency.

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[61] R stands for unknown other components.

Table 22 Fire sizes and their frequencies for risk calculation

Fire size	Oxygen supply	Frequency of occurrence (/yr)
20 m^2	Not restricted	$0.00088 \times 0.89 = 7.83 \times 10^{-4}$
50 m^2	Not restricted	$0.00088 \times 0.09 = 7.92 \times 10^{-5}$
100 m^2	Not restricted	$0.00088 \times 0.01 = 8.8 \times 10^{-6}$
300 m^2	Not restricted	$0.00088 \times 0.005 = 4.4 \times 10^{-6}$
900 m^2	Not restricted	$0.00088 \times 0.005 = 4.4 \times 10^{-6}$

As the oxygen supply is not restricted, the combustion rate for a warehouse containing 75 wgt% flammable liquids is equal to 0.081 $kg/m^2 \cdot s$. The resulting source terms are presented in Table 23. The toxic products are released into the recirculation zone of the building and subsequently disperse further downwind at a constant height (i.e. without lifting off).

Table 23 Source terms for the different fire sizes

Parameter	20 m^2	50 m^2	100 m^2	300 m^2	900 m^2
Release duration (s)	600	600	600	1800	1800
Combustion rate (kg/s)	1.63	4.06	8.13	24.38	73.13
NO_2 production rate (kg/s)	0.05	0.13	0.27	0.80	2.40
HCl production rate (kg/s)	0.17	0.42	0.84	2.51	7.52
SO_2 production rate (kg/s)	0.32	0.81	1.62	4.87	14.61

The ‘average Dutch’ wind rose in SAFETI-NL was used to calculate consequence and risk distances. This wind rose uses a predefined set of weather conditions for day- and night-time. The relative occurrences of these weather conditions are shown in Table 24. These occurrences are further divided over 12 different wind directions. The most frequent wind direction is from the south-south-west.

Table 24 Relative probability of atmospheric conditions used for the risk calculation

Atmospheric stability	Wind speed	Daytime	Night-time
Pasquill class B	3 m/s	0.09	
Pasquill class D	1.5 m/s	0.05	0.08
Pasquill class D	5 m/s	0.13	0.14
Pasquill class D	9 m/s	0.17	0.15
Pasquill class E	5 m/s		0.06
Pasquill class F	1.5 m/s		0.13

SAFETI-NL 8.21 was used to calculate consequence and risk distances. Figure 12 shows the 10^{-6} and 10^{-7} individual risk contours. The largest distance from the edge of the warehouse to the individual risk level of 10^{-6} per year is 40 metres. This largest distances to the individual risk levels of 10^{-7} and 10^{-8} per year are 270 m and 830 m, respectively.

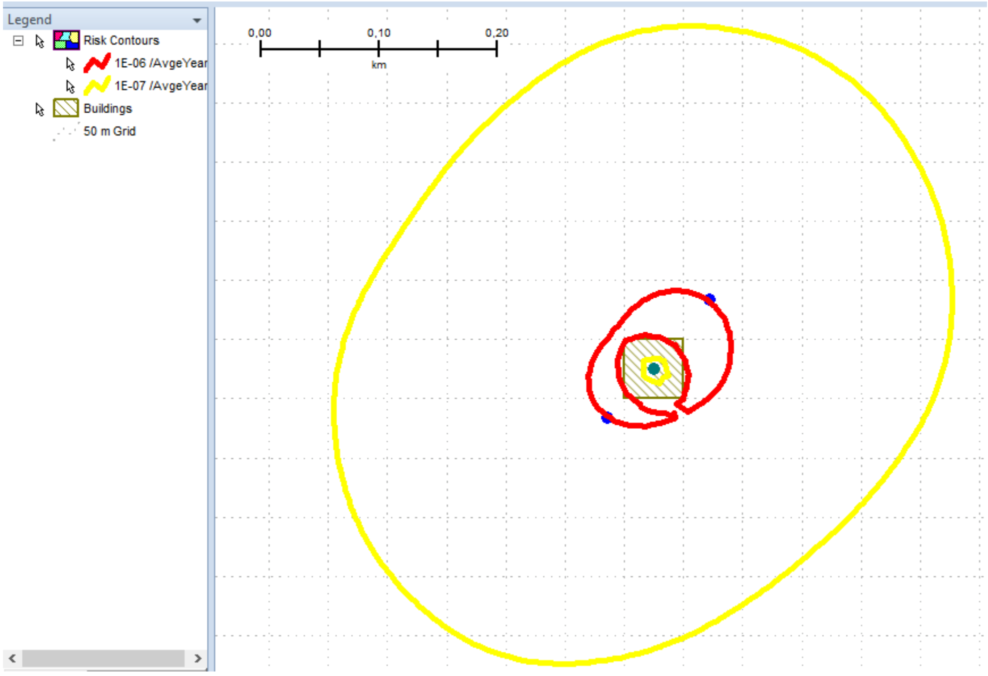

Figure 12 Individual risk contours for the reference warehouse (zoomed in on risk level 10^{-7} per year)

Two sets of consequence distances are presented in Table 25; the 1% lethality distance and the maximum distance to 192 ppm. Both distances are calculated from the downwind side of the building. The concentration 192 ppm is used to determine the area in which protective measures for persons near hazardous activities should be considered [8].[62]

- The maximum 1% lethality distance is 2 km and occurs for fire size 900 m^2 and weather conditions F1.5 (stable weather with a wind speed of 1.5 m/s).
- The maximum distance to 192 ppm is almost 5 km from the edge of the building and occurs for the same fire size and weather.

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[62] The area where safety measures should be considered is the area where indoor exposure to toxic products can be life-threatening. Presuming a 30-minute scenario duration and a building ventilation rate of 1 volume per hour, an outdoor concentration of 192 ppm will result in an indoor concentration of 75 ppm. 75 ppm is the ‘life-threatening concentration’ of nitrogen dioxide for exposure duration 30 minutes. Between the different toxic combustion products, nitrogen dioxide has the lowest life threatening concentration. Life-threatening concentrations for different exposure durations were derived by a group of Dutch toxicologists [19].

Table 25 Summary of consequence distances for the reference warehouse (distance from the downwind side of the building)

Fire size	**Weather class**	**Maximum distance to 1% lethality (m)**	**Maximum distance to 192 ppm (m)**[63]
20 m^2	B3	n/a	n/a
	D1.5	n/a	45
	D5	n/a	n/a
	D9	n/a	n/a
	E5	n/a	n/a
	F1.5	n/a	30
50 m^2	B3	n/a	50
	D1.5	n/a	100
	D5	n/a	n/a
	D9	n/a	n/a
	E5	n/a	n/a
	F1.5	n/a	180
100 m^2	B3	n/a	80
	D1.5	55	275
	D5	n/a	65
	D9	n/a	25
	E5	n/a	65
	F1.5	50	650
300 m^2	B3	80	200
	D1.5	250	850
	D5	65	240
	D9	n/a	100
	E5	65	375
	F1.5	700	2400
900 m^2	B3	190	500
	D1.5	800	2000
	D5	230	750
	D9	95	450
	E5	350	1200
	F1.5	2100	4900

When examining the dispersion in SAFETI-NL in detail, it became clear that the plume centreline height remains close to the ground for all combinations of fire size and wind speed. This is because possible lift-off is supressed in the modelling if the building wake option is selected. Consequently, downwind concentrations are overpredicted if buoyancy is significant, i.e. if the fire size is large and/or the wind speed small.

Figure 13 shows the dimensionless buoyancy flux for the different fire sizes and wind speeds. For this calculation, a convective energy per unit mass of 2 MJ/kg was assumed. The combustion rate is defined by the fraction of flammable liquids in the warehouse and is equal to 0.081 $kg/m^2{\cdot}s$. The dimensionless buoyancy flux is assumed to be equal to $8.9{\cdot}Q_{conv}$.

Note: For compact releases, the effect of buoyancy becomes significant if the dimensionless buoyancy flux $F/(u^3{\cdot}H)$ is above 0.11 (see Section

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[63] The reported SAFETI-NL distances apply to a toxic averaging time of 600 s. This is the default value.

3.5.5). For distributed releases, effects of buoyancy will become significant about one order of magnitude later. In Figure 13, the dimensionless buoyancy flux is expressed in terms of $F/(u^3 \cdot W)$. The building width will generally be at least twice the building height: $F/(u^3 \cdot W) \leq ½ \cdot F/(u^3 \cdot H)$.

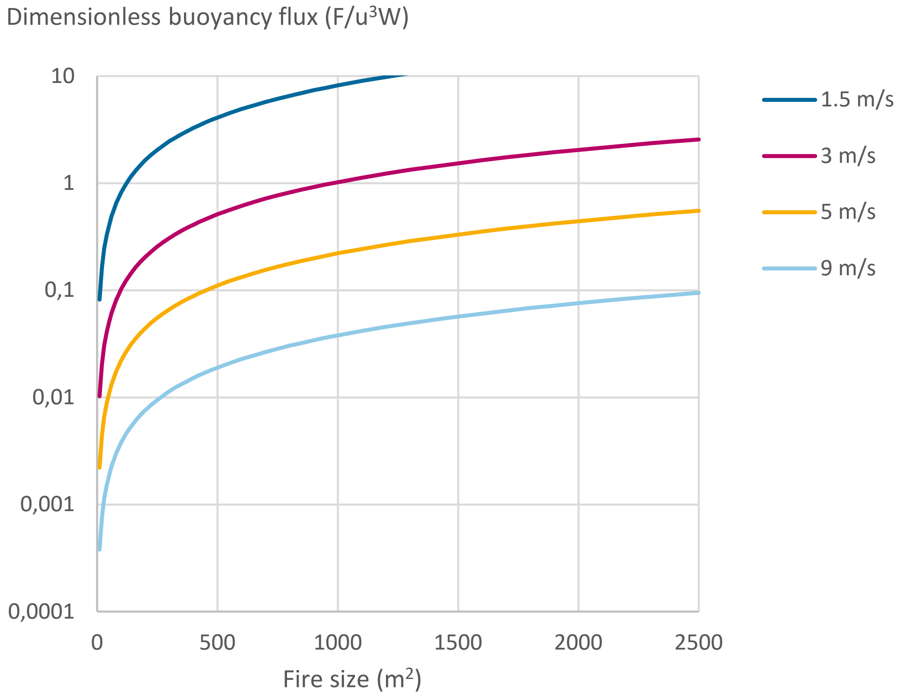

Figure 13 Dimensionless buoyancy flux as a function of fire size for combustion rate 0.081 kg/m²·s and convective heat per unit mass 2 MJ/kg

5.1.2 *Validity of the results*

The validity of the calculated consequence distances is tested by comparing these results with predictions from the HBC correlation (Section 3.5.5.1) and the AB correlation (Section 3.6.4). Together, these two correlations are assumed to define the possible range of outcomes (Section 4.5).

5.1.2.1 Outcomes for Hanna, Briggs and Chang and Atkinson and Briggs

The predicted concentrations for the HBC and AB correlations are presented prior to comparing these with SAFETI-NL outcomes.

The following assumptions were used to generate these graphs:

- The assumed combustion rate per unit area depends on the fraction of flammable liquids stored in the warehouse and is equal to 0.081 kg/s·m².
- The convective heat fraction is assumed to be 2 MJ/kg. This value is expected to be a low value for real fires.[64] The calculated ground-level concentrations are then conservative.

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[64] Average heats of combustion and average convective heat fractions were reported in Table 15 for different types of materials. The average heat of combustion was between 14 and 47 MJ/kg and the average convective heat fraction between 0.36 and 0.6. The resulting convective heat would then be between 5 and 28 MJ/kg.

- The toxic release rate is the sum of the release rates for NO_2, SO_2 and HCl. Using the average substance composition and the existing conversion factors, the toxic release rate is 0.34 times the combustion rate (i.e. 0.027 kg/s·m^2).
- The average molecular mass for the NO_2, SO_2, HCl mixture is 0.054 kg/mol. This average mass is used to convert concentrations in kg/m^3 to ppm.

Figure 14 shows the predicted concentrations as a function of fire size for wind speed 1.5 m/s. Three downwind distances are plotted in the graph.

- For both correlations, the calculated concentrations are well below 192 ppm for all fire sizes.
- With HBC (dotted lines), the concentrations rapidly reduce with increasing fire size. This is a result of the increasing buoyancy with fire size.
- With AB (solid lines), the calculated concentrations are stable between fire sizes 200 m^2 and 1000 m^2. This means that the increase in toxic release rate with fire size and the increase in buoyancy flux with fire size are in balance in this range.

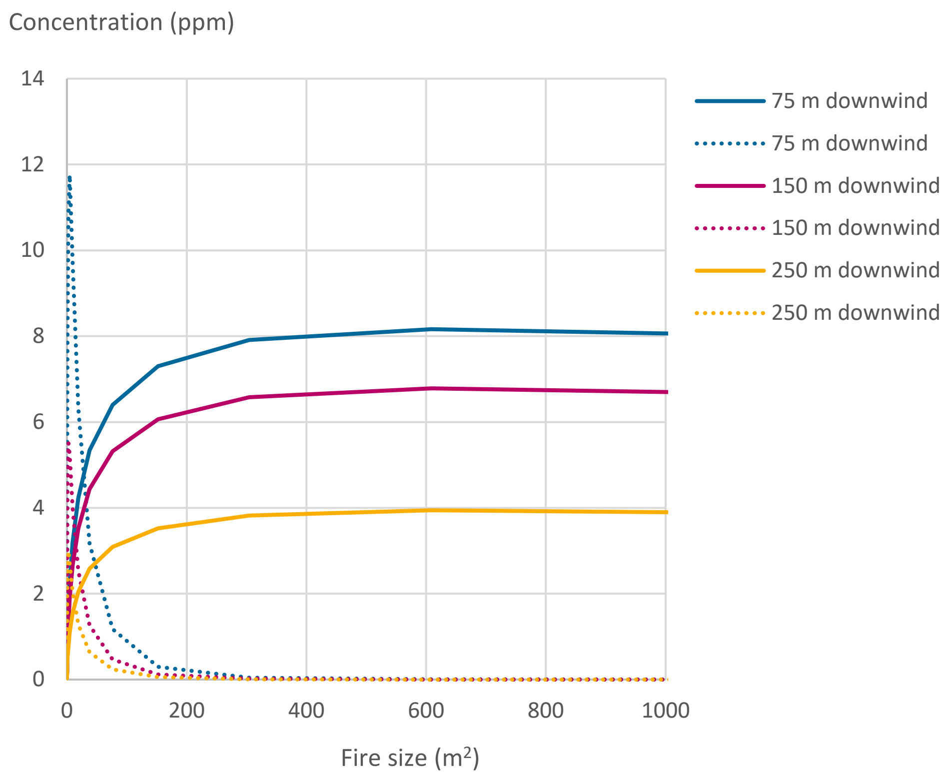

Figure 14 Downwind concentrations predicted by the AB (solid lines) and HBC (dotted lines) correlations for the reference case for wind speed 1.5 m/s

However, the data in Table 15 represented well-ventilated fires and did not account for heat losses to the building. Heat losses to the building can be between 60% and 90% for a well-developed fire prior to roof collapse (see Section 3.4.3).

Overall, the two correlations show very different trends. As was discussed in Section 4.5, the HBC correlation appears to apply to compact releases with limited mixing in the recirculation zone, whereas the AB correlation applies to distributed releases that fully mix in the recirculation zone. Plume lift-off is much more significant when using the first correlation. This result in much smaller ground-level concentrations for most fire sizes.

Figure 15 shows the predicted concentrations as a function of fire size for wind speed 9 m/s. Again, three downwind distances are plotted in the graph.

- The concentrations for 9 m/s (Figure 15) are all larger than those for 1.5 m/s (Figure 14). This is a result of the reduced buoyancy by the increased wind speed.
- For HBC (dotted lines), the ground-level concentrations initially increase with fire size due to the higher toxic release rate and later reduce due to the increased buoyancy. Up to a downwind distance of 150 m, the concentration can exceed the critical value of 192 ppm. Beyond 150 m, the concentration is 100 ppm or less.
- The AB correlation (solid lines) results in ground-level concentrations well below 192 ppm. This is a result of the more significant mixing in the recirculation zone (compared with HBC). The calculated concentrations increase with fire size. The largest concentrations are found if the fire size is equal to the full storage size.

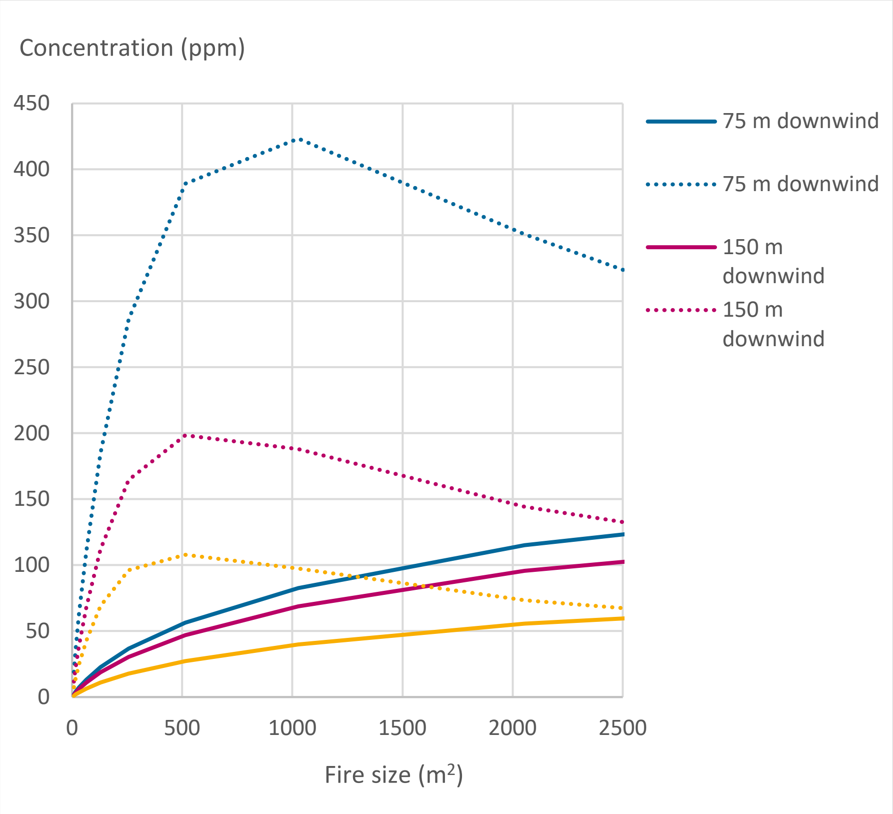

Figure 15 Downwind concentrations predicted by the AB (solid lines) and HBC (dotted lines) correlations for the reference case for wind speed 9 m/s

Together, Figure 15 and Figure 14 show that the differences between the two correlations can be significant. Which correlation gives the greater ground-level concentrations depends on fire size and wind speed.

5.1.2.2 Comparison with SAFETI-NL outcomes

In Table 26, distances to outdoor concentration 192 ppm are compared between the existing Dutch method (Table 25) and predictions from the HBC correlation (equation 21) and of AB correlation (equation 27). 'N/A' indicates that the calculated concentrations are below 192 ppm everywhere downwind of the building. The fire sizes and weathers used in this table are those required by the Dutch method.

Table 26 Maximum distances to concentration 192 ppm and corresponding fire size (between brackets)

Weather	Existing NL method	Hanna, Briggs and Chang	Atkinson and Briggs
B3	500 m (900 m^2)	15 m (90 m^2)	N/A
D1.5	2000 m (900 m^2)	N/A	N/A
D5	750 m (900 m^2)	55 m (200 m^2)	N/A
D9	450 m (900 m^2)	160 m (600 m^2)	N/A
E5	1200 m (900 m^2)	55 m (200 m^2)	N/A
F1.5	4900 m (900 m^2)	N/A	N/A

The following observations can be made from Table 26:

- For the existing NL method, the maximum distance to 192 ppm always corresponds to fire size 900 m^2. Because buoyancy effects are not accounted for in the existing Dutch method (because the building-wake model is selected), the largest fire size will always provide the largest consequence area. Overall, the largest distance is obtained for stable weather with low wind speed (F1.5). This distance is 4900 m.
- For all weathers, the HBC correlation results in smaller distances to 192 ppm. The fire size that produces the largest distance for this correlation is always smaller than 900 m^2. This is a result of the more significant buoyancy of large fire sizes. At some point below 900 m^2, the effect of increasing buoyancy is stronger than the effect of the increasing toxic mass release rate.
- The AB correlation results in concentrations downwind of the building below 192 ppm for all fire sizes and weathers. For small fire sizes, the toxic release rate is too low to provide a concentration of 192 ppm in the recirculation zone. For large fire sizes, the combination of mixing in the recirculation zone and reduced ground-level concentrations due to buoyancy leads to concentrations below 192 ppm.

Table 26 demonstrates that the existing Dutch method indeed gives overconservative outcomes. This is most prominent for a wind speed of 1.5 m/s.

5.2 Ways of accounting for the effect of buoyancy

The current method does not consider the effects of buoyancy on downwind dispersion. In the current subsection, different ways of improving the method in this respect are investigated.

- Option 1 is to define a new model in SAFETI-NL specifically adapted to warehouse fires. Such a model should be able to capture both mixing in the recirculation zone and lift-off due to buoyancy. An advanced model would distinguish between the fraction of the release that is captured in the recirculation zone and the fraction that remains above the recirculation zone.
- Option 2 is to mimic realistic plume dispersion in the existing version of SAFETI-NL with suitable input parameters. In order to allow the plume to lift off, the building-wake model cannot be used in this option. When deselecting the building-wake model, buoyancy effects can be accounted for by increasing the release temperature.
- Option 3 is to try to obtain realistic downwind ground-level concentrations by reducing the source term that is used as input for the calculations. The reduction of the source term should depend on the expected reduction of ground-level concentrations due to buoyancy. This option is a workaround, as it tries to counter inaccurate (or invalid) dispersion outcomes by reducing the source term.
- Option 4 is to implement an on/off criterion for lift-off. Below a critical fire size, buoyancy is assumed to be low enough to ignore. Above the critical value, lift-off is assumed to be so large that ground-level concentrations will no longer be relevant for consequence and risk calculations. The critical fire size should depend on wind speed and building characteristics. This method is used in Flanders (see Section 3.6.1).

In the following subsections the four ways of improving the method are illustrated and discussed. In the last subsection (5.3) the conclusions are presented.

5.2.1 *Option 1: Implementing a dedicated warehouse fire model in SAFETI-NL*

The first option is to define a new model in SAFETI-NL specifically adapted to warehouse fires. Such a model should be able to capture both mixing in the recirculation zone and lift-off due to buoyancy. Such an advanced model would distinguish between the fraction of the release that is captured in the recirculation zone and the fraction that remains above the recirculation zone.

No specific detailed models for dispersion related to warehouse fires were found in the literature. Several features of the dispersion of smoke from building fires were discussed in publications by David Hall et al. and in reviews of studies on building fire dispersion [53], [55]. Some of the publications discussed in these reviews focused on plume centreline height, while others focused on ground-level concentrations. No methods were found that discuss all elements of 3D dispersion (plume height, plume width and plume depth). Moreover, the latest series of wind tunnel experiments by David Hall et al. [49] identified that dispersion is different for compact releases and distributed releases. Correlations found in the literature do not distinguish between these two release geometries. Information about the influence of the building orientation in relation to the wind and about the influence of the location of the release in the building is also limited.

Hanna, Briggs and Chang [59] combined tests for compact releases and distributed releases into a single correlation. The behaviour of this correlation is very similar to that of compact releases. This suggests that the number of distributed releases that was used to obtain the correlation was much smaller than the number of compact releases. Hanna, Briggs and Chang provided a correlation only for downwind concentrations on the projected plume axis (centreline). Therefore, the correlation cannot be used to identify in what two-dimensional area concentrations can be exceeded.

Atkinson and Briggs [32] proposed correlations for ground-level centreline concentration and plume width. Therefore, their work makes it possible to identify in what area specific ground-level concentrations can be exceeded. Atkinson and Briggs used only runs for distributed releases to obtain their correlation. A comparison with the work by Hanna, Briggs and Chang showed that the AB correlation may underpredict ground-level concentrations if the release is compact and if the dimensionless buoyancy flux is below 0.1. A single building size was used by AB to derive their correlation: width 25 m, length 75 m and height 10 m. It is unknown how reliable the correlation is for buildings of different dimensions.

The ADMS model used by Atkinson and Briggs was not analysed in detail. Detailed analysis of that model could be part of future work.

Modifying SAFETI-NL will take at least two years. It first needs to be determined in detail how the modelling needs to be modified. No readily available options are available in open literature today. The code must then be produced, verified, validated and tested before it can be added to the software. The timeline also depends on other (independent) enhancements of the software.

5.2.2 *Option 2: Mimicking plume lift-off by deselecting the building-wake model in SAFETI-NL*

The existing Dutch method prescribes that the ‘Roof/Lee’ building-wake model in SAFETI-NL should be used for consequence calculations. A side-effect of this requirement is that possible lift-off effects after mixing in the building wake are suppressed by the software. It was shown in Section 5.1.2.2 that this shortcoming in the model behaviour results in unrealistic (overconservative) outcomes.

In this subsection, it is investigated whether current SAFETI-NL outcomes can be made more realistic if the building-wake model is not used. The underlying idea is that the influence of plume lift-off is more important than that of mixing in the recirculation zone. Plume lift-off depends on the convective heat contained by the source term. This convective heat is defined by the volume flux of the release and the average temperature of this volume flux. It should therefore be investigated which combination of source term and release temperature gives acceptable outcomes.

SAFETI-NL uses the density of the plume to evaluate the rise or descent of the plume if the building-wake model is not used. Releases at high temperature will lift-off from the ground. As a result, it is no longer desirable to use a maximum fire size of 900 m^2.[65] The ground-level concentrations that are now calculated by the program, depend on mass release rate, release temperature and weather conditions. The user can identify which combination of fire size and weather gives the largest ground-level concentrations downwind from the source.

5.2.2.1 Source term equal to the toxic mass release rate

The first test is to use the existing source term for dispersion calculations, which is the toxic mass release rate. The toxic mass release rate is the sum of the release rates for nitrogen dioxide (NO_2), sulphur dioxide (SO_2) and hydrogen chloride (HCl) (see Section 5.1.1). The toxic mass fraction in the smoke plume is less than 10%.

Outcomes of runs in SAFETI-NL with different release temperatures were compared with predictions of the HBC and AB correlations. These outcomes are presented in detail in Appendix 2 and summarised below. For the two correlations, the inputs and outcomes are identical to those presented in Section 5.1.2.

The main observations are:

- Simply deselecting the 'Roof/Lee' building-wake model in SAFETI-NL resulted in critical errors. To avoid these errors, the different warehouse scenarios needed to be converted manually into user-defined scenarios. The conversion is time-consuming and susceptible to errors and therefore not recommended for standard users. In a future version of SAFETI-NL, the modification of scenarios could be automated.
- The release temperature was varied between a slightly elevated temperature of 50 ^{0}C and the maximum allowed temperature of 600 ^{0}C. A higher release temperature results in lower ground-level concentrations, due to enhanced lift-off of the plume. The highest temperature (600 ^{0}C) gave the best fit with the HBC and AB correlations. This may not be surprising, as the source term (equal to the toxic mass release rate) is much smaller than the total smoke production rate, in this option. The deficit in volume flux then needs to be compensated by a relatively high release temperature.
- Table 27 shows the calculated distances for SAFETI-NL, using a release temperature of 600 ^{0}C, and for the two correlations. The outcomes for the two correlations are identical to those previously reported (Table 26).
- For all wind speeds, the SAFETI-NL distances are larger than those of the HBC correlation. The difference is particularly large for weather F1.5. This can be explained by the way in which the interaction with the inversion layer is modelled.[66] This outcome (distance 1750 m) is not deemed realistic.
- For all wind speeds, the largest SAFETI-NL distances are obtained if the fire size is equal to its maximum (2500 m^2). Using the HBC

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[65] The maximum fire size of 900 m^2 was a workaround to ignore fire sizes which were supposed to result in significant plume rise. The critical value (900 m^2) lacked scientific underpinning, see Chapter 2.

[66] In SAFETI-NL, the maximum centreline height is capped by the height of the inversion layer. For weather F1.5, an inversion layer height of 50 m is assumed. The plume depth increases with distance. As the volume flux of the plume is significant, the plume eventually returns to ground level. This is deemed an undesired effect of the cap applied to the maximum centreline height.

correlation, the most conservative fire size is wind-speed-dependent, and normally substantially smaller than 2500 m^2.
- Using the AB correlation, the predicted downwind concentration is below 192 for all combinations of fire size and weather (see Section 5.1.2.2).

Table 27 SAFETI-NL distances to 192 ppm for the release of NO_2, SO_2 and HCl and using a release temperature of 600 ⁰C, compared with the HBC and AB correlations (convective heat per unit mass 2 MJ/kg)

Weather	**SAFETI-NL (T = 600⁰)**	**Hanna, Briggs and Chang**	**Atkinson and Briggs**
B3	150 m (2500 m^2)	15 m (90 m^2)	n/a
D1.5	n/a	n/a	n/a
D5	240 m (2500 m^2)	55 m (200 m^2)	n/a
D9	325 m (2500 m^2)	160 m (600 m^2)	n/a
E5	210 m (2500 m^2)	55 m (200 m^2)	n/a
F1.5	1750 m (2500 m^2)	n/a	n/a

The conclusion of this first test is that the outcomes of SAFETI-NL have reduced when compared with the current method but, compared with the two reference correlations, the calculated distances are still substantially larger.

5.2.2.2 Source term equal to the sum of all combustion products and entrained nitrogen

In the solution above, the source term for dispersion was equal to the sum of the production rates of three toxic combustion products: NO_2, HCl and SO_2. In reality, the smoke released from a fire has many more components, including N_2, CO_2, H_2O, CO and soot.[67] The combustion rate and mass release rates for different components of the smoke plume are listed in Table 28. These data apply to the warehouse and the fuel composition that were described in Section 5.1 and are subject to the following additional assumptions:

- There is no shortage of oxygen. As a result, the fire is 'fuel-restricted' and the total combustion rate is the product of the predefined combustion rate per unit area (0.081 kg/m^2·s) and the fire size.
- All oxygen in the fuel is consumed by the fire.
- 10% of the nitrogen is converted into NO_2; all other nitrogen is converted into other nitrous gases.
- 95% of the carbon is converted into CO_2 and 5% into CO.
- The nitrogen entrainment rate is determined by the oxygen demand rate (which defines the amount of air consumed) and the fraction of nitrogen in air.
- The convective energy per unit mass of fuel is between 2 and 8 MJ/kg. For a fuel with an effective combustion energy of 20 MJ/kg, this would mean that 10–40% of the combustion energy is conserved as convective energy.

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[67] The effect of soot is currently ignored. Soot increases the density of the plume and thereby reduces buoyancy. If hot soot particles are deposited on the ground, convective energy is removed from the smoke plume. This also reduces the buoyancy of the plume.

- The smoke temperature prior to dilution is determined by the convective energy (MW) and the total mass release rate of combustion products and nitrogen (kg/s). Coherent with the convective energy, the temperature is presented as a range of outcomes.
- The specific heat capacity of the smoke is equal to that of air at ambient temperature (1006 J/kg·K) and the molar weight of the smoke (combustion products and nitrogen) is equal to 0.030 kg/mole. The smoke temperature does not depend on fire size because the assumed fraction of energy converted into convective energy does not depend on fire size.

Table 28 Main characteristics of the fire dynamics and the smoke composition

Parameter	**Fire size 100 m²**	**Fire size 300 m²**	**Fire size 900 m²**
Combustion rate per unit area (kg/m²·s)	0.081	0.081	0.081
Total combustion rate (kg/s)	8.13	24.4	73.1
Convective energy (MW)	16–65	49–195	146–585
Mass rate for NO_2 (kg/s)	0.27	0.80	2.41
Mass rate for SO_2 (kg/s)	1.63	4.89	14.7
Mass rate for HCl (kg/s)	0.84	2.51	7.52
Mass rate for CO (kg/s)	0.27	0.82	2.45
Mass rate for CO_2 (kg/s)	8.13	24.4	73.2
Mass rate for H_2O (kg/s)	3.61	10.8	32.5
Mass rate for other substances (kg/s)	2.81	8.42	25.3
Oxygen consumption rate (kg/s)	9.27	27.8	83.4
N_2 entrainment (kg/s)	32.5	97.4	292
Total mass release rate (kg/s)	50	150	450
Estimated smoke temperature prior to dilution (°C)	343–1312	343–1312	343–1312

The data in Table 28 provide only an indication of the numbers involved. The numbers depend considerably on the assumptions made for fire size, combustion rate, fuel composition and emission factors.

It can be derived from Table 28 that undiluted smoke consists of approximately 65 wgt% nitrogen, 16 wgt% carbon dioxide and 7 wgt% water. The combined fraction of NO_2, SO_2 and HCl in undiluted smoke is 5.5 wgt%. The fraction of CO is 0.5 wgt%. When ignoring nitrogen, carbon dioxide, water and other products in the smoke, the mass flux is significantly underestimated. For higher accuracy, it is therefore recommended to define a plume containing all substances (toxic and non-toxic) and to correct the concentration of interest for the toxic fraction in the plume.

Outcomes of runs in SAFETI-NL with different release temperature were compared with predictions of the HBC and AB correlations. These outcomes are presented in detail in Appendix 2 and summarised below.

For the two correlations, the inputs and outcomes are identical to those presented in Section 5.1.2.

The main observations are:

- As before (Section 5.2.2.1), the different warehouse scenarios needed to be converted manually into user-defined scenarios. Such a conversion is time-consuming and susceptible to errors and not recommended for standard users. In a future version of SAFETI-NL, the modification of scenarios could be automated.
- Compared with the previous test (Section 5.2.2.1), plume lift-off was more significant if the same release temperatures was used. This makes sense because the volume flux is now substantially larger than before.
- The release temperature was varied between 50 ⁰C and 250 ⁰C. A higher release temperature results in lower ground-level concentrations, due to enhanced lift-off of the plume. Overall, a release temperature of 100 ⁰C gave the best fit with the concentrations to 192 ppm predicted by the HBC and AB correlations.
- Table 29 shows the calculated distances for SAFETI-NL, using a release temperature of 100 ⁰C and for the two correlations. The outcomes for the two correlations are identical to those previously reported (Table 26).
- For all wind speeds, the SAFETI-NL distances are comparable to or larger than those for the HBC correlation. However, the differences have reduced and the agreement is better than before (cf. Section 5.2.2.1). The large distance for weather F1.5 is caused by unrealistic modelling of the interaction with the inversion layer and is not deemed realistic.
- Again, the largest SAFETI-NL distances are obtained if the fire size is equal to its maximum (2500 m^2). Using the HBC correlation, the most conservative fire size is wind-speed-dependent, and in all cases much smaller than 2500 m^2.
- Using the AB correlation, the predicted downwind concentration is below 192 for all combinations of fire size and weather (see Section 5.1.2.2).

Table 29 SAFETI-NL distances to 192 ppm for the release of the entire smoke plume and using a release temperature of 100 ⁰C, compared with HBC and AB correlations (convective heat per unit mass 2 MJ/kg)

Weather	**SAFETI-NL (T = 100⁰)**	**Hanna, Briggs and Chang**	**Atkinson and Briggs**
B3	55 m (2500 m^2)	15 m (90 m^2)	n/a
D1.5	5 m (2500 m^2)	n/a	n/a
D5	55 m (2500 m^2)	55 m (200 m^2)	n/a
D9	170 m (2500 m^2)	160 m (600 m^2)	n/a
E5	50 m (2500 m^2)	55 m (200 m^2)	n/a
F1.5	1500 m (2500 m^2)	n/a	n/a

The conclusion of this second test is that the outcomes of SAFETI-NL have further reduced. Compared with the first test, the calculated distances show better agreement, in particular with the outcomes of the HBC correlation.

5.2.2.3 Discussion

Distances to a concentration of 192 ppm were calculated using two different modelling options. In the first test, the volume flux was made equal to the toxic mass release rate. In the second test, the volume flux was made equal to the sum of all combustion gases.
The calculated distances were compared with the distances calculated using the HBC and AB correlations. The latter correlation resulted in concentrations below 192 ppm for all fire sizes and weathers, and was therefore not very useful for comparison.[68]

Distances to 192 ppm reduced substantially when deselecting the building-wake option and using elevated release temperatures. In the first test, a release temperature of 600 ºC gave the best agreement with distances calculated with the HBC and AB correlations. In the second test, a release temperature of 100 ºC gave the best agreement. In both tests, the calculated distances were still larger than those calculated using the HBC correlation.

Notes of concern:

- The two correlations that were used for comparison both have limitations. The HBC correlation was derived from a set of wind tunnel experiments for compact and distributed releases. Compact releases appear to have been dominant in this dataset. The correlation is likely to overestimate buoyancy for distributed releases, thereby underpredicting the ground-level concentrations for these releases away from the recirculation zone. The AB correlation was derived from a series of numerical runs for distributed releases from the roof of a building. It may underestimate centreline concentrations if the release is not fully mixed in the recirculation zone of the building.
- Related to the above, the two correlations result in substantially different concentration profiles (see Section 5.1.2.1). Away from the recirculation zone, the difference can be up to a factor of 5. Within the recirculation zone, the difference can be even larger than a factor of 5.
- The focus on the distance to 192 ppm hides further differences in concentration profiles. Even if the calculated distance to 192 ppm is similar to that obtained with a correlation, it is likely that the concentration at other distances will show less agreement.
- The comparison was carried out for a single reference case, which is not representative of the entire set of chemical warehouses in The Netherlands. The level of agreement for other warehouses is unknown.
- The scenario input in SAFETI-NL was time-consuming and susceptible to errors. This work could, however, be automated in a future version of SAFETI-NL.

Given the above concerns, the possible solution presented in this subsection does not provide enough assurance that concentration profiles for different fire sizes and weathers will be calculated sufficiently

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[68] A comparison of concentration profiles would have been more useful but requires presentation of a larger set of outcomes. This high level of detail was not deemed desirable for the main part of the report. In Appendix 2, concentration profiles for the different methods used are provided and discussed.

realistically. Option 2 is therefore not deemed suitable as a modification of the Dutch risk method.

5.2.3 *Option 3: Reducing the source term to account for buoyancy*

Option 3 is to investigate whether the source term in SAFETI-NL can be reduced in order to compensate for the effect of buoyancy. Investigations earlier in this report have shown that the precise effect of buoyancy on releases in the wake of a building is uncertain. The effect was much smaller when using the AB correlation than with the HBC correlation. As the former is more conservative, it is used to further explore Option 3.

Equation 27 gives the AB correlation for ground-level concentrations as a function of downwind distance (x) and buoyancy number (F'). The latter is the product of the dimensionless buoyancy flux and the constant Π: $F' = \Pi \cdot F/(u^3 W)$. $F' = 0.001$ is the lower end of the validation range for equation 27 and $C(0.001)$ can be regarded as the ground-level concentration in absence of buoyancy. [69]

The reduction factor $f_{\text{reduction}}$ is equal to the ratio of the ground-level concentration for a buoyant release and the ground-level concentration for a non-buoyant release. Using equation 27 and equation 29, we can write:

$$
\begin{aligned}
f_{\text{reduction}} &= \frac{C(F')}{C(0.001)} \\
&= \frac{0.17 \cdot \frac{\dot{m}_{\text{tox}}}{u\,W^2}\left(\frac{W}{x}\right)^{1.2} \cdot f(F')}{0.17 \cdot \frac{\dot{m}_{\text{tox}}}{u\,W^2}\left(\frac{W}{x}\right)^{1.2} \cdot f(0.001)} \\
&= \frac{f(F')}{f(0.001)} \\
&= \frac{10^{-\left(0.7 \cdot log_{10} F' + 0.12 \cdot (log_{10} F')^2\right)}}{10.47}
\end{aligned}
\tag{39}
$$

As can be observed from equation 39, the reduction factor only depends on buoyancy number (dimensionless buoyancy flux) if the AB correlation is used. It needs to be determined for all different combinations of combustion rate (convective heat) and wind speed.

Once the reduction factor has been determined for a combination of combustion rate and wind speed, the source term for that combination must be modified accordingly. This requires the use of user-defined scenarios in SAFETI-NL. In this section however, we only examine the largest effect distances for ground-level concentration 192 ppm. These could be found by identifying the worst-case fire size for each wind speed and calculating the corresponding reduction factor for ground-level concentrations (equation 39). The worst-case fire size is the fire size that has a buoyancy number of 5.7 (see Section 3.6.4.2.1), or the

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[69] This approach is a little complicated because equation 29 is not a monotonically decreasing function. It reaches a maximum when F′=0.0012. Furthermore, its maximum is not 1 but 10.49. It was therefore decided to normalise outcomes to *F′*= 0.001, i.e. f(F′) = 10.47.

maximum size of the storage (usually the size of the fire compartment) if that size is smaller. The resulting effect distances were calculated in two ways, which produced almost identical outcomes.[70]

The maximum effect distances for Option 3 are reported in Table 30, along with the worst-case fire sizes and reduction factors per wind speed (weather class). The largest distance to 192 ppm is 220 m and corresponds to weather D9 and fire size 2500 m^2 (entire floor area). The second and third largest distances are obtained for D5 and E5, respectively. The agreement with the outcomes of the HBC and AB correlations is similar to that of test 2 in the previous subsection (see Table 29).

Table 30 Fire sizes and maximum effect distances for Option 3

Weather class	**Worst-case fire size (m^2)**	**Corresponding buoyancy number *F'***	$f_{reduction}$	**Distance to 192 ppm (m)**
B3	1761	5.66	0.024	45
D1.5	220	5.66	0.024	n/a
D5	2500	1.74	0.064	95
D9	2500	0.30	0.207	220
E5	2500	1.74	0.064	110
F1.5	222	5.70	0.024	n/a

Similar to Option 2 (Section 5.2.2), Option3 also requires the use of user-defined scenarios in SAFETI-NL. The user-defined scenarios are specific for each combination of combustion rate and wind speed. Again, the conversion is time-consuming, susceptible to errors and not recommended for standard users. In a future version of SAFETI-NL, the modification of scenarios could be automated.

A disadvantage of Option 3 is that the proposed modification factor is obtained indirectly via the AB correlation (equation 27). Equation 27 involved a fit to limited number of numerical runs in a computer code for a single warehouse configuration. As such, equation 27 is not deemed robust enough to use for different warehouse configurations.

5.2.4 *Option 4: Defining a critical fire size and neglecting buoyancy effects*

In this fourth option, the effect of buoyancy is assumed to be on/off. For fire sizes below a critical value, the dispersion is assumed to be neutral (without buoyancy effects). Above the critical value, plume rise is assumed to be sufficiently large to exclude these fire sizes from consequence and risk calculations. A similar approach is used in Flanders (Section 3.6.1). The only difference from the approach used in Flanders is that fire size in the current proposal is not restricted to a maximum of 900 m^2.

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[70] The first way of modelling was to use a modified fire size for input in SAFETI-NL. The modified fire size was the product of the worst-case fire size (per wind speed) and the corresponding reduction factor. This is a valid workaround because the mass production rata is proportional to the fire size (if the combustion rate is fuel restricted) and the ground-level concentrations are proportional to the mass production rate (if the dispersion is neutral). The second way of modelling was to use default inputs but to divide the concentration of interest (192 ppm) by the reduction factor. The differences between the two ways of modelling were negligible. In both calculations, the assumed combustion rate per unit area was 0.081 kg/m^2·s and the assumed convective heat per unit mass of fuel 2 MJ/kg. It was further assumed that the buoyancy flux is equal to 8.5·Q.

In this option, the HSE [63] lift-off criterion $\frac{F}{u^3 \cdot H} = \frac{8.9 \cdot Q_{conv}}{u^3 \cdot H} \geq 0.18$ (equation 25) is used to identify when lift-off is assumed to be sufficiently large[71]. This criterion can be rewritten as:

$$Q_{\mathrm{conv}} \geq \frac{0.18 \cdot u^3 \cdot H}{8.9} \qquad (40)$$

where Q_{conv} is expressed in MW.

Scenarios will be included in the consequence and risk calculation only if the convective heat (Q_{conv}) is smaller than the critical value $\frac{0.18 \cdot u^3 \cdot H}{8.9}$. The convective heat depends on fire size, the average combustion rate per unit area and the average convective heat per unit fuel mass. As the latter two parameters are assumed to be constant, the criterion essentially gives a maximum fire size for consequence and risk calculations.

Table 31 shows the maximum fire size per weather class for the reference scenario and the corresponding effect distances.

- The largest fire size is found for weather D9 and is equal to 1243 m^2. The maximum fire size for D5 and E5 is 213 m^2. Fire sizes for other weathers are below 50 m^2.
- It should be noted that these maximum fire sizes depend on the assumed combustion rate per unit area (0.081 kg/m^2·s) and the assumed convective heat per unit mass (2 MJ/kg). The maximum fire sizes will be a factor of 3.25 higher if the combustion rate is 0.025 kg/m^2·s (and the convective heat 2 MJ/kg).
- The largest distance to 192 ppm is 600 m. This distance is obtained for weather D9. For weathers D1.5 and F1.5 (wind speed 1.5 m/s), the concentrations in the wake of the building and further downwind are below 192 ppm.
- The maximum fire sizes are slightly larger than the modified fire sizes for worst-case scenarios of Table 30. This suggests that Option 4 is slightly more conservative than Option 3. This is also reflected in the calculated effect distances, which are slightly larger in Option 4 than in Option 3.

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[71] Assuming that the building has a width to height ratio between 2 and 4, the corresponding critical dimensionless buoyancy flux expressed in terms of F/u^3W is somewhere between 0.05 and 0.1.

Table 31 Maximum fire sizes and maximum effect distances for Option 4

Weather class	**Maximum fire size (m²)**	**Distance to 192 ppm (m)**
B3	46	45
D1.5	6	n/a
D5	213	130
D9	1243	600
E5	213	200
F1.5	6	n/a

The proposed solution (Option 4) has the following advantages:

- The maximum fire size depends on wind speed, which is physically realistic.
- The approach is fairly easy to comprehend and does not depend on too many different physical parameters.
- The criterion is certainly suitable for compact releases. For compact releases, David Hall concluded that reductions of one order of magnitude occur when the dimensionless buoyancy flux F/u^3H is around 0.11. The proposed criterion (0.18) is slightly above that value. David Hall also concluded that ground-level concentrations rapidly reduce with further increase of buoyancy flux.
- The resulting consequence distances are smaller than those calculated by the current method, but still larger (sometimes considerably larger) than those reported for the HBC and AB correlations (see Section 5.1.2.2). In other words, the solution is moving in the right direction but is still conservative.

A disadvantage is that the solution uses an on/off criterion, while the literature shows that the effects of lift-off increase gradually with buoyancy.

A note of concern is that it has not yet been demonstrated that the criterion is also suitable for distributed releases. At the same time, the AB correlation, which applies to distributed releases, resulted in concentrations below 192 ppm for almost all the scenarios and warehouse configurations considered in this report. Caution can be built into this option by using a low value for the amount of convective energy produced per kg of fuel. In this chapter, a value of 2 MJ/kg was assumed. That value is equal to the value used in the Flemish risk method (Section 3.6.1). Atkinson and Briggs [32] assumed a value of 10 MJ/kg, which appears to be high (see Section 3.4.3 and footnote 64).

5.3 Summary and recommendation

Four of improving the modelling in SAFETI-NL were investigated.

From a scientific point of view, the preferred option is to improve the dispersion modelling in SAFETI-NL by including a dedicated model for smoke dispersion from building fires (Option 1). This requires additional research. It is expected that developing such a model will take at least two years.

Options 2, 3 and 4 are simplifications and should be regarded as possible workarounds for ‘getting the dispersion right’.

Option 2 was to mimic plume rise by using an elevated release temperature and by suppressing mixing in the building wake. Consequence distances to 192 ppm were reduced and were in better agreement with the distances obtained with the correlations from literature than the current distances. However, several concerns were raised (Section 5.2.2.3). For example, it was not investigated whether the modification also resulted in better outcomes for other concentrations or other warehouses. Given the concerns, Option 2 does not appear to be a good way forward.

Option 3 involved a reduction of the source term to compensate for the reduction of ground-level concentrations due to buoyancy. The reduction factor was deduced from the AB correlation. With the reduced source term, consequence distances reduced to values similar to those in Option 2. A disadvantage of this option was that the proposed reduction factor (equation 39) was obtained from a correlation that was fitted to a set of numerical runs for a single warehouse configuration and was therefore not deemed robust enough to use for detailed modelling in a future version of the Dutch risk method.

Option 4 was to limit consequence calculations to a maximum (critical) fire size, and to assume passive dispersions for all fire sizes up to this critical size. The consequence distances for this option were somewhat larger than those calculated for Options 2 and 3, but still significantly smaller than those obtained with the current method. An advantage of Option 4 is that the proposed criterion was reported in literature and that it is also used in Flanders.

Considering the above, it is recommended to choose between Option 1 and Option 4.

6 Conclusions and recommendations

6.1 Introduction

It was investigated whether the existing Dutch method for the risk assessment of chemical warehouses should be updated. For this investigation, the assumptions underlying this method were reiterated in the different sections of Chapter 2. A literature survey was carried out to identify the best available scientific practices today (Chapter 3). By comparing the two, several options for improvement to the current method were identified (Chapter 4). Different ways of accounting for building and buoyancy effects were investigated in Chapter 5.

A lot of uncertainties apply when assessing the toxic risk of chemical warehouse fires. To name a few:

- The products stored in warehouses vary with time and it is difficult to obtain representative storage data.
- Fire spread and fire intensity depend on the types of packaging used, the stack height and the availability of oxygen. These variables may change in time, may vary between different parts of the fire compartment and may change during the cause of the fire.
- Automatic fire suppression systems can limit fire growth but may not be activated or fail in their response. The actual response of the fire suppression system is unknown prior to the fire.
- Production rates of toxic components depend on combustion efficiency, which depends on the fire intensity and the availability of oxygen. They will vary during the cause of the fire and are difficult to predict with great accuracy.
- Emissions from the building depend on the size, number and location of openings in the building. The emissions will also vary during the cause of the fire and are also difficult to predict with great accuracy.
- Subsequent dispersion depends on the wind speed, the interaction of the building with the wind and the convective energy that is conserved in the plume. The number of possible variations is large.

In the light of these uncertainties, it is deemed impossible to calculate risks and effects with great accuracy. Calculation methods can provide only rough estimates of the off-site risk and of the distances over which significant health effects can be expected.

Fire scenarios are created to represent the many different ways in which a fire can progress. In many cases, four or five fire sizes and two ventilation regimes need to be considered. A scenario duration and a relative probability are defined for each combination. Specific values used in the current method were obtained in the late 1980s and early 1990s by expert judgement and lack scientific underpinning. The level of detail is high when considering the different uncertainties in fire development. A possible way forward is to reduce the level of detail in the fire scenarios to be used.

6.2 Warehouse fire frequency

The validity of the figure for warehouse fire frequency was discussed in Section 4.2. The fire frequency used in the current risk method is substantially lower than two values that were reported in the literature.

6.3 Fire development

The validity of the assumptions used for the development of a fire was discussed in Section 4.3. It was observed that fire development is complex and dependent on many parameters. The complexity is increased if the effects of fire suppression, or failure thereof, also need to be accounted for. In the Dutch method, the effects of fire suppression and its possible failure are accounted for by using specific fire size distributions per type of fire suppression. This approach is sophisticated but has little scientific underpinning.

A possible way forward is to reduce the level of detail in the fire scenarios to be used. Automatic fire suppression systems can fail entirely or partly or can be fully effective. No calculations are needed if the suppression is fully effective. As a result, the method should distinguish between complete or partial failure of automatic fire suppression. To avoid unwarranted precision, one fire size can be used for each type of failure.

In the absence of automatic fire suppression systems, the local fire brigade will not try to extinguish the fire in the compartment. These fires will therefore eventually consume the entire fire compartment. Thus, only one fire size is needed for risk and consequence estimation.

The largest fire size to be used should further depend on the buoyancy of plumes and the amount of lift-off that is expected. This topic is discussed in Section 6.5.

6.4 Combustion rate

The validity of the combustion rates that are calculated with the current method was discussed in Section 4.4. The current method distinguishes between a fuel-restricted combustion rate and an oxygen-restricted combustion rate. Though physically correct, it provides a false sense of precision, as both combustion rates are calculated in a simplistic manner. It is recommended to investigate whether the calculation method can be simplified by considering only the fuel-restricted combustion rate. This is a conservative approach. Adding further detail to the method is not recommended, as the required input parameters will remain uncertain.

In addition, the fuel-restricted combustion rate for high-rack storages should be further investigated. If the amounts of flammable solids (ADR class 4) and/or oxidising substances (ADR class 5) can be significant in chemical warehouses, the fuel-restricted combustion rates of these substances should also be investigated further.

6.5 Effects of buildings and buoyancy on ground-level concentrations

The effects of buildings and buoyancy on ground-level concentrations were discussed in Section 4.5 and were further investigated in

Chapter 5. The main observation was that the current method does not properly account for plume rise. The current method uses a maximum fire size of 900 m^2 and does not consider any effects of plume rise for any fire size. In reality, plume rise depends on building dimensions and wind speed. For low wind speeds, plume rise can be significant if the fire size is well below 900 m^2. For the largest wind speed, 9 m/s, plume rise may only be significant if the fire size is larger than 900 m^2.

Four ways of improving the dispersion modelling were investigated in Section 5.2, with a short summary in Section 5.3. Two of these solutions (Option 2 and Option 3) were not deemed to be sufficiently robust. The remaining options are to define a new model in SAFETI-NL that is specifically adapted to warehouse fires (Option 1) or to limit consequence calculations to a maximum (critical) fire size and assume neutral dispersions for all fire sizes up to this critical size (Option 4). The latter is a workaround for defining a new dispersion model. The development of a new model (Option 1) will take at least two years. Option 4 does not require new model development and can be easily implemented. The outcomes for Option 4 were deemed sufficiently reliable in the light of the significant uncertainties related to dispersion modelling for buoyant releases from buildings.

6.6 Accounting for other toxic combustion products

This topic was discussed in Section 4.7. Currently, only three toxic combustion products are considered in the risk calculation method: nitrogen dioxide, sulphur dioxide and hydrogen chloride. Emissions of carbon monoxide are not yet considered, but can be significant. A conversion factor for carbon to carbon monoxide of 0.05 appears to be reasonably conservative. Release rates of hydrogen fluoride are normally insignificant and can be added to the release rate of hydrogen chloride as in the current approach. This may, however, not apply when large numbers of Li-ion batteries are stored in a warehouse.

6.7 Effects of exposure to toxic substance

The calculation of the toxic effects of exposure to toxic substances was discussed in Section 4.8.

- The probit values that are currently used are outdated. New values are available that have a better scientific underpinning.
- For mixtures of toxic substances, the likelihood of fatality related to exposure to the mixture is calculated as if the different components in the mixture were independent. This assumption is not deemed realistic.
- The effect contour represents the area where the lowest 'life-threatening value' of any of the toxic products can be exceeded. This approach might be too conservative if the fraction of this 'most toxic' component in the mixture is small.

6.8 Recommendations

The following recommendations emerged from the investigation:

1. There is an indication that the warehouse fire frequency is underestimated in the current Dutch method. It is therefore recommended that this frequency be updated. Despite unsuccessful attempts in the past, it is assumed that sufficient

data are now available to determine a new warehouse fire frequency.

2. The number of scenarios to be used in the risk calculation is large and many underlying parameters (fire sizes, ventilation rates, scenario durations and relative probabilities) lack adequate underpinning. In the light of the various uncertainties, it is recommended that the method be simplified by reducing the number of scenarios to be used in the risk calculation.
3. The calculation of the combustion rate can also be simplified by considering only the fuel-restricted combustion rate. This is a conservative approach and reduces the false sense of precision that the current method provides.
4. The way in which the buoyancy of the release is accounted for should be improved. From a scientific point of view, the preferred solution is to develop a new dedicated model for smoke dispersion from building fires in SAFETI-NL (Option 1). A workaround would be to identify a largest fire size with insignificant plume lift-off (Option 4). This largest fire size would depend on building dimensions and wind speed. The Flemish lift-off criterion (equation 40) is expected to provide reasonable results.
5. Emissions of carbon monoxide should also be considered. The fraction of carbon that will be converted into carbon monoxide is around 0.05.
6. The recently derived probit values should be used to determine the likelihood of fatality for exposure to toxic substances.
7. For exposure to a mixture of toxic substances, it is recommended to improve the method for calculating the likelihood of fatality and the method for identifying the representative life-threatening concentration.

List of symbols

Symbol	**Description and SI units**[72]
Latin symbols	
A	Fire size (area), in m^2
A_0	Area of opening (for ventilation-controlled fires), in m^2
B	Combustion rate per unit area in $kg/m^2 \cdot s$
C	Concentration, normally in kg/m^3
c_p	Specific heat capacity in $J/kg \cdot K$
f_{ADR3}	Mass fraction of ADR class 3 flammable liquids
F	Buoyancy flux in m^4/s^3
F^*	Dimensionless buoyancy flux
F'	Buoyancy number (dimensionless)
g	Gravitational acceleration constant in m/s^2
H	Building height, in m
H_0	Height of opening (for ventilation-controlled fires), in m
H_c	Ideal heat of combustion per unit mass, in J/kg
H_{conv}	Convective energy released per unit mass of fuel, in J/kg
H_{eff}	Effective heat of combustion per unit mass of fuel, in J/kg
H_{rad}	Radiative energy released per unit mass of fuel, in J/kg
L_p	Lift-off parameter
$\dot{m}$	Combustion rate, in kg/s
$\dot{m}_a$	Air mass flow rate (for ventilation-controlled fires), in kg/s
$\dot{m}_{FR}$	Fuel-restricted combustion rate (i.e. combustion rate in excess of air), in kg/s
$\dot{m}_{OR}$	Oxygen-restricted combustion rate (i.e. combustion rate in excess of air), in kg/s
$\dot{m}_{\mathrm{p}}$	Mass release rate for toxic component p, in kg/s
$\dot{m}_{\mathrm{tox}}$	Toxic mass release rate, in kg/s
Q	Heat release rate, in W
Q_{conv}	Convective heat flux, in W
r	stoichiometric air–fuel mass ratio
t	Time, normally in s
T_a	Ambient air temperature (at 1.5 m height), in K
u	wind velocity, in m/s
u_*	Atmospheric friction velocity, in m/s
V_s	Source volume emission rate (at emission temperature), in m^3/s
W	Building width, in m
x	Downwind distance, in m
y_p	Mass loss yield of toxic component p, dimensionless
Greek symbols	
α	Fire growth rate for t^2-model, in kW/s^2
ρ_a	Ambient air density in kg/m^3
ρ_s	Smoke density (at elevated temperature), in kg/m^3
σ_y	Standard deviation of the Gaussian concentration profile in lateral direction, in m

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[72] Units are specified in the report and can deviate from the SI units. For example, energy can be expressed in J, kJ, MJ or GJ and mass can be expressed in grams or kilograms.

Symbol	**Description and SI units**[72]
σ_Z	Standard deviation of the Gaussian concentration profile in vertical direction, in m
χ_{conv}	Convective energy fraction
χ_{eff}	Combustion efficiency
χ_{rad}	Radiative energy fraction

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Appendix 1 Search terms used in Scopus search

Scopus was used to find relevant scientific papers. The search for papers was carried out in February 2017. In August 2021, the search was carried out once again to check that any new papers (published between 2017 and 2021) were included. In addition, the fourth search term was modified from 'toxic AND impact' to 'toxic' alone, to obtain a larger number of results.

Date	**Search string**	**Number of results**
14-2-2017	TITLE-ABS-KEY (chemical AND warehouses) AND TITLE-ABS-KEY (fire) AND ALL (dispersion)	12
20-2-2017	TITLE-ABS-KEY (warehouse AND fire AND dispersion)	17
20-2-2017	TITLE-ABS-KEY (warehouse AND fire AND plume)	28
20-2-2017	TITLE-ABS-KEY (warehouse AND fire AND toxic AND impact)	13
18-8-2021	(TITLE-ABS-KEY (chemical AND warehouses) AND TITLE-ABS-KEY (fire) AND ALL (dispersion)) OR (TITLE-ABS-KEY (warehouse AND fire AND dispersion)) OR (TITLE-ABS-KEY (warehouse AND fire AND plume)) OR (TITLE-ABS-KEY (warehouse AND fire AND toxic AND impact))	60
18-8-2021	(TITLE-ABS-KEY (chemical AND warehouses) AND TITLE-ABS-KEY (fire) AND ALL (dispersion)) OR (TITLE-ABS-KEY (warehouse AND fire AND dispersion)) OR (TITLE-ABS-KEY (warehouse AND fire AND plume)) OR (TITLE-ABS-KEY (warehouse AND fire AND toxic))	84

Appendix 2 Outcomes when not using the building-wake model in SAFETI-NL (Option 2)

It was explored in Section 5.2.2 whether the outcomes from SAFETI-NL would improve if the building-wake model was deselected (Option 2). Not using the building-wake model has the advantage that the dispersion model considers buoyancy effects if the density of the plume is less than that of ambient air. Two tests were carried out:

1. Modelling the release of NO_2, HCl and SO_2 at elevated temperature (without using the building-wake option).
2. Modelling the release of all combustion products and entrained nitrogen at elevated temperature (without using the building-wake option).

Test 1: Modelling the release of the toxic combustion products NO_2, HCl and SO_2 without the building-wake model

In this test, the building-wake model in SAFETI-NL was not used. Instead, the release is modelled as a point source, using user-defined scenarios. The source term is equal to the sum of the three standard toxic combustion products, NO_2, HCl and SO_2, and depends on fire size (see Table 23). Thus, it represents only a small fraction of the total smoke plume. The release height (7 m) is assumed to be half the building height (13.7 m). When applying the HBC and AB correlations, it is assumed that the convective heat per unit mass is 2 MJ/kg.

Figure 16 shows the side view of the modelled dispersion in SAFETI-NL. The figure represents the release related to a fire of 900 m^2 for weather D9. It can be seen that plume lift-off is larger for higher release temperatures. Increasing the release temperature from 50 ºC to 250 ºC has a small effect on the maximum distance to 192 ppm at ground level. Increasing the release temperature further to 600 ºC has a more significant effect for this case.

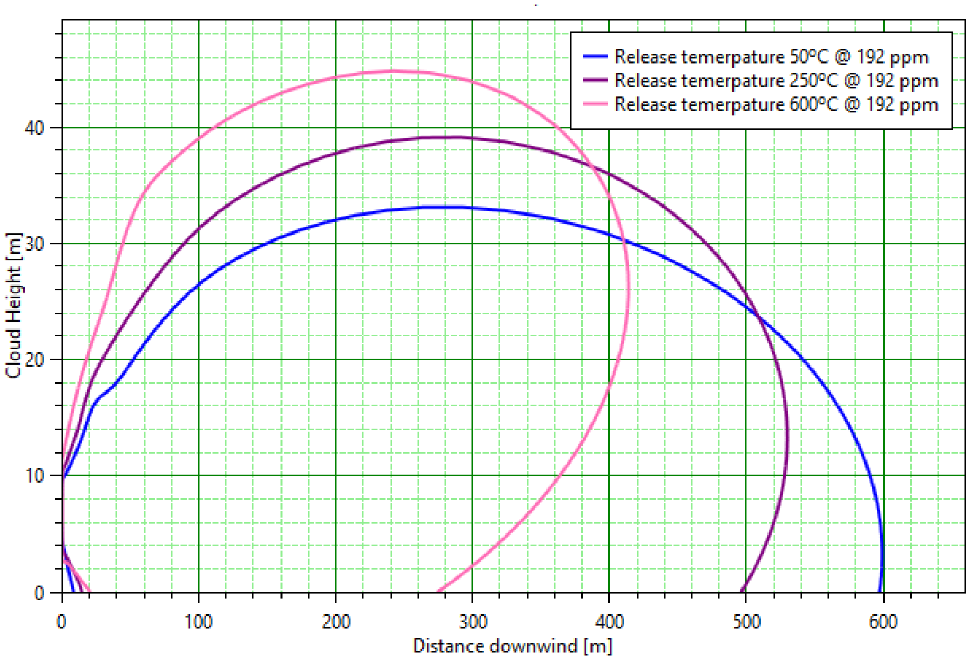

Figure 16 Side view of the smoke plume in SAFETI-NL for weather D9 and fire size 900 m^2, for three different release temperatures and with building-wake option deselected. Summed concentration of NO_2+HCl+SO_2 equal to 192 ppm.

In Figure 17, the ground-level concentrations from SAFETI-NL are compared with the correlations of Hanna, Briggs and Chang and of Atkinson and Briggs. The fire size and wind speed are the same as before (900 m^2 and 9 m/s). The ground-level concentrations that are calculated with SAFETI-NL are higher than those predicted by the HBC and AB correlations. The closest fit applies to the highest release temperature used: 600 ºC. A better fit cannot be obtained, as the maximum release temperature that can be used in SAFETI-NL is just above 600 ºC.

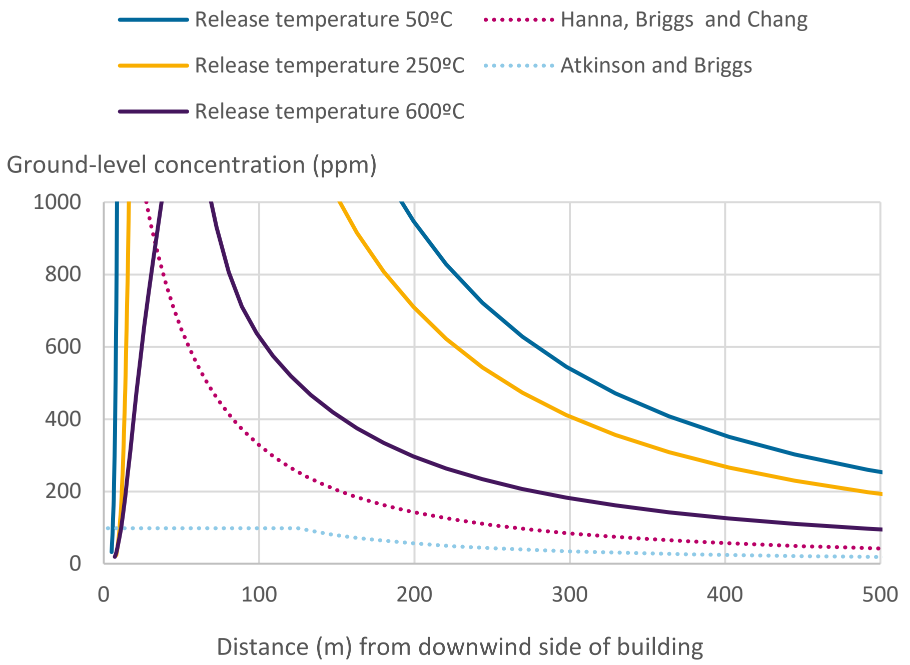

Figure 17 Ground-level concentration of NO_2+HCl+SO_2 for fire size 900 m^2 in absence of building-wake model for wind speed 9 m/s, compared with HBC and AB correlations

Another observation from Figure 17 is that the HBC correlation yields higher concentrations than the AB correlation. In the recirculation zone (downwind distance smaller than 125 m), the difference is a factor of 3 or more. Downwind of the recirculation zone, the difference is roughly a factor of 2.

The outcomes of the first test are compared with the outcomes of the HBC and AB correlations (Table 32).

- For all wind speeds, the SAFETI-NL distances are larger than those of HBC. The difference is particularly large for weather F1.5. This can be explained by the way in which the interaction with the inversion layer is modelled.[73] This outcome (distance 1750 m) is not deemed realistic.
- For all wind speeds, the largest SAFETI-NL distances are obtained if the fire size is equal to its maximum (2500 m^2). Using HBC, the most conservative fire size is wind-speed-dependent, and normally substantially smaller than 2500 m^2.
- Using the AB correlation, the predicted downwind concentration is below 192 for all combinations of fire size and weather (see Section 5.1.2.2).

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[73] In SAFETI-NL, the maximum centreline height is capped by the height of the inversion layer. For weather F1.5, an inversion layer height of 50 m is assumed. The plume depth increases with distance. As the volume rate of the plume is significant, the plume eventually returns to ground level. This is deemed an undesirable effect of the cap applied to the maximum centreline height.

Table 32 SAFETI-NL distances to 192 ppm for the release of NO_2, SO_2 and HCl and using a release temperature of 600 ⁰C, compared with HBC and AB correlations

Weather	**Parameter**	**Suggested approach (T = 600 ⁰C)**	**Hanna, Briggs and Chang**	**Atkinson and Briggs**
B3	Max. distance to 192 ppm	150 m	15 m	n/a
	Corresponding fire size	2500 m^2	90 m^2	n/a
D1.5	Max. distance to 192 ppm	n/a	n/a	n/a
	Corresponding fire size	n/a	n/a	n/a
D5	Max. distance to 192 ppm	250 m	55 m	n/a
	Corresponding fire size	2500 m^2	200 m^2	n/a
D9	Max. distance to 192 ppm	325 m	160 m	n/a
	Corresponding fire size	2500 m^2	600 m^2	n/a
E5	Max. distance to 192 ppm	210 m	55 m	n/a
	Corresponding fire size	2500 m^2	200 m^2	n/a
F1.5	Max. distance to 192 ppm	1750 m	n/a	n/a
	Corresponding fire size	2500 m^2	n/a	n/a

Test 2: Modelling the entire smoke plume while not using the building-wake model

In this test, the release is again modelled as a point source, using user-defined scenarios in SAFETI-NL. The building-wake model in SAFETI-NL is again not used. Contrary to the previous test, the source term is now equal to the sum all combustion products and additional nitrogen that is entrained in the plume. The total release rate is noted in Table 23. The release height is again assumed to be equal to the building height.

Figure 18 shows the side view of the plume for a plume concentration of 5670 ppm, which is the equivalent of a concentration of 192 ppm for NO_2, SO_2 and HCl alone. As expected, the plume lift-off increases with the release temperature used. Lift-off is also more substantial compared with modelling the release of toxic combustion products alone (see Figure 16).

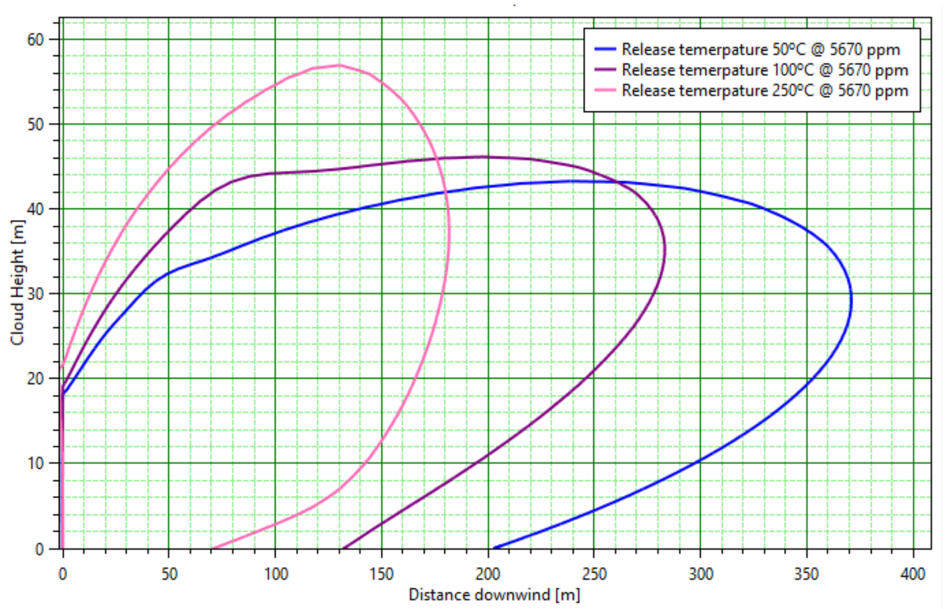

Figure 18 Side view of the dispersion of the entire smoke plume for weather D9 and fire size 900 m^2 with building-wake option deselected

Figure 19 shows the concentration as a function of downwind distance for the same inputs. The outcomes of the HBC and AB correlations are the same as before (Figure 17). The use of a release temperature of 50 ^{0}C gives higher concentrations than predicted by the HBC and AB correlations. The outcomes for a release temperature of 100 ^{0}C are close to the HBC correlation and higher than the AB correlation. For a release temperature of 250 ^{0}C, the SAFETI-NL outcomes are in between those of the two correlations.

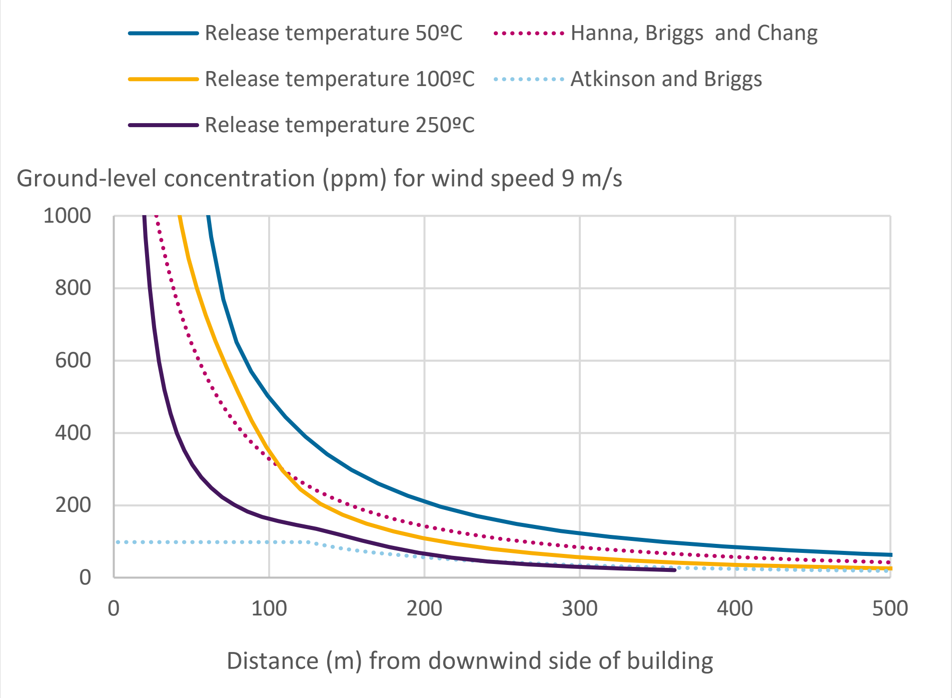

Figure 19 Combined NO_2, SO_2 and HCl concentration for wind speed 9 m/s and fire size 900 m^2, using the entire smoke plume in the source term for SAFETI-NL

The outcomes of the second test are compared with the outcomes of the HBC and AB correlations in Table 33. The reported distance are measured from the downwind side of the building.

- For some wind speeds, the SAFETI-NL distances are larger than those from HBC, while for other weathers, the SAFETI-NL distances are smaller. The difference is particularly large for weather F1.5. This can be explained by the way in which the interaction with the inversion layer is modelled.[74] This outcome (distance 1500 m) is not deemed realistic.
- For all wind speeds, the largest SAFETI-NL distances are obtained if the fire size is equal to its maximum (2500 m^2). Using HBC, the most conservative fire size is wind-speed-dependent, and in all cases substantially smaller than 2500 m^2.
- Using AB, the predicted downwind concentration is below 192 for all combinations of fire size and weather (see Section 5.1.2).

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[74] In SAFETI-NL, the maximum centreline height is capped by the height of the inversion layer. For weather F1.5, an inversion layer height of 50 m is assumed. The plume depth increases with distance. As the volume rate of the plume is significant, the plume eventually returns to ground level. This is deemed an undesirable effect of the cap applied to the maximum centreline height.

Table 33 SAFETI-NL distances to 192 ppm for the release of the entire smoke plume using a release temperature of 100 ⁰C, compared with the HBC and AB correlations

Wind speed	**Parameter**	**Suggested approach (T = 100⁰)**	**Hanna, Briggs and Chang**	**Atkinson and Briggs**
B3	Max. distance to 192 ppm	55 m	15 m	n/a
	Corresponding fire size	2500 m^2	90 m^2	n/a
D1.5	Max. distance to 192 ppm	5 m	n/a	n/a
	Corresponding fire size	2500 m^2	n/a	n/a
D5	Max. distance to 192 ppm	55 m	55 m	n/a
	Corresponding fire size	2500 m^2	200 m^2	n/a
D9	Max. distance to 192 ppm	170 m	160 m	n/a
	Corresponding fire size	2500 m^2	600 m^2	n/a
E5	Max. distance to 192 ppm	50 m	55 m	n/a
	Corresponding fire size	2500 m^2	200 m^2	n/a
F1.5	Max. distance to 192 ppm	1500 m	n/a	n/a
	Corresponding fire size	2500 m^2	n/a	n/a

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