

# Spill behaviour using REACTPOOL Part I. Results for accidental releases of chlorosulphonic acid ( $\text{HSO}_3\text{Cl}$ )

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## Abstract

Chlorosulphonic acid is a toxic, highly reactive and corrosive substance that exists in its liquid form at ambient conditions. Its major hazardous potential comes from the clouds of hydrogen chloride and sulphuric acid mist produced whenever this chemical escapes from containment and is exposed to moisture. It decomposes violently and sometimes explosively in the presence of water, liberating heat. On spillage it creates liquid pools that can either boil or evaporate. There are three sources of water available for reaction: free ground water, substrate water and atmospheric moisture. Hydrogen chloride gas or aqueous solution and sulphuric acid liquid are produced by the hydrolysis reaction.

This paper describes the dangers involved in cases of accidental releases of chlorosulphonic acid, referring to its properties, toxicity data and mitigation tests. It also reports results of pool behaviour using REACTPOOL [T. Kapias, R.F. Griffiths, C. Stefanidis, *J. Haz. Mat.*, submitted for publication]. These results indicate that the pool behaviour is governed mainly by the amount of water available for reaction. Surface roughness and wind speed also have a significant effect on the results. A discussion of the results in comparison with those for other water reactive substances is presented in Part III of this series of papers [T. Kapias, R.F. Griffiths, *J. Haz. Mat.*, submitted for publication]. The generated cloud will initially contain chlorosulphonic acid, hydrogen chloride and sulphuric acid with numerous processes taking place. Initially, it is usually denser than air.

Although chlorosulphonic acid has been involved in major hazard incidents, there are no experimental data relevant to the modelling requirements. Use of REACTPOOL provides insights into the major hazard role of this substance. © 2001 Elsevier Science B.V. All rights reserved.

*Keywords:* Spill behaviour; Chlorosulphonic acid; REACTPOOL

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## 1. Introduction

$\text{HSO}_3\text{Cl}$  contains equimolar quantities of  $\text{HCl}$  and  $\text{SO}_3$ . It is referred to in the literature as chlorosulphonic acid as well as chlorosulphuric acid, or simply CSA. Its potential to cause harm to people and the environment has been recognised by its inclusion in many items of national and international legislation [1–3]. It resembles sulphur trioxide in its behaviour and properties, although it is generally described as less toxic than  $\text{SO}_3$ .

On escape from containment it creates liquid pools, usually on land. It is highly hygroscopic and reacts readily and exothermically with any available water. The pool will contain  $\text{H}_2\text{SO}_4$  and  $\text{HSO}_3\text{Cl}$  or excess water, and its composition and properties will continuously change as  $\text{HSO}_3\text{Cl}$  reacts with water generating  $\text{H}_2\text{SO}_4$  liquid and  $\text{HCl}$  gas. It may boil or evaporate depending mainly on the amount of water available for reaction (there is no possibility of solidification). Water is supplied to the pool from three sources: there is free ground water, substrate water and atmospheric moisture.  $\text{H}_2\text{SO}_4$  will also attack concrete or asphalt surfaces and will react with some of their compounds [4]. The pool behaviour has been incorporated into REACTPOOL [5] and some preliminary scenarios were examined [6]. Model results indicate that it is mainly affected by the amount of water available for reaction. Surface roughness and wind speed also have a significant effect [7].

The generated cloud will initially contain  $\text{HCl}$  gas,  $\text{HSO}_3\text{Cl}$  and small quantities of  $\text{H}_2\text{SO}_4$  vapours.  $\text{HSO}_3\text{Cl}$  will continuously react with atmospheric moisture yielding  $\text{H}_2\text{SO}_4$  and  $\text{HCl}$  vapour and gas respectively, eventually being fully consumed.  $\text{H}_2\text{SO}_4$  and  $\text{HSO}_3\text{Cl}$  vapour will also interact with atmospheric moisture yielding aerosols. Some of the vapour and aerosol will be deposited on the ground due to gravitational settling and other deposition mechanisms. In many cases the generated cloud will initially be denser than air. Only after some distance downwind, allowing adequate dilution with air, will it become passive. Overall, the behaviour of the generated cloud is very complex as it will initially contain three components in different phases (vapour and aerosols). Even after some distance downwind, it will contain  $\text{HCl}$  gas and  $\text{H}_2\text{SO}_4$  aerosol. Its behaviour resembles the behaviour of clouds generated from spills of  $\text{SO}_3$  and oleum with the additional complexity that a third component,  $\text{HCl}$ , is involved.

A survey of accidents involving water reactive chemicals that occurred in the USA in the period 1990–1999 showed that there is about one accident per year in the USA involving spillage of  $\text{HSO}_3\text{Cl}$  [5].

Although  $\text{HSO}_3\text{Cl}$  has been involved in some major hazard incidents no theoretical or experimental published data on its release behaviour could be found. The only experiments that have been conducted were to test the effectiveness of different methods on mitigating and suppressing fumes generated from such spills.

## 2. Uses and properties

$\text{HSO}_3\text{Cl}$  is a colourless, mobile, extremely reactive liquid with a pungent odour. It fumes very strongly in air and has been used as a military smoke-generating agent. Its main uses

Table 1  
Main properties of HSO<sub>3</sub>Cl [8–11]

Property	Value
Molecular weight (kg kmol <sup>-1</sup> )	424–432
Boiling point (K)	193
Freezing point (K)	700
Critical temperature (K)	85
Critical pressure (bar)	195
Critical volume (cm <sup>3</sup> mol <sup>-1</sup> )	1753
Liquid density at 20°C (kg m <sup>-3</sup> )	452–460
Heat of vaporisation (kJ kg <sup>-1</sup> )	0.016
Vapour pressure at 30°C (atm)	2.6
Viscosity at 20°C (cP)	1.18
Specific heat at 15–80°C (kJ kg <sup>-1</sup> K <sup>-1</sup> )	116.53

are in organic synthesis as a sulphating, sulphonating or chlorosulphonating agent. Its applications are principally as an intermediate in the production of synthetic detergents, drugs and dyestuffs. It is preferred in some applications because it is a strong sulphonating agent but is less destructive than SO<sub>3</sub>. It is non-flammable, but it may cause ignition on contact with combustible materials. Heating beyond its boiling point results in decomposition into sulphur dioxide, chlorine and water [8–11].

Some of its properties are reported in Table 1. Further details are given in Appendix A.

### 3. Toxicity data and mitigation tests

No specific studies on testing toxicity effects of HSO<sub>3</sub>Cl for humans have been conducted. HSO<sub>3</sub>Cl liquid is a severe irritant of the eyes and skin [12–14]. The vapour is extremely irritating to the eyes, skin, lung and mucous membranes. The following acute (short-term) health effects may occur immediately or shortly after exposure to HSO<sub>3</sub>Cl [14].

- Severe skin and eye irritation and burns leading to permanent eye damage.
- Nose and throat problems causing coughing and wheezing.
- Irritation of the lungs, causing coughing and/or shortness of breath. Higher exposures can cause a build-up of fluid in the lungs (pulmonary oedema), a medical emergency, with severe shortness of breath.

In respect of its chronic (long-term) effects, repeated exposures may cause severe irritation of the lungs, and the development of bronchitis with cough, phlegm, and/or shortness of breath [14].

From an animal study it was observed that respiratory tract and ocular irritation occurred, with histopathological changes in internal organs in acutely poisoned animals. According to this study, the inhalation LC50 in mouse was reported to be 52 mg m<sup>-3</sup> for 2 h exposure, while in rats it was 38.5 mg m<sup>-3</sup> for 4 h [15].

Occupational exposure standards have been set for HSO<sub>3</sub>Cl in the USA as follows:

- Emergency Response Planning Guidelines (ERPG) [16]:

- ERPG(1) =  $2 \text{ mg m}^{-3}$  (no more than mild, transient effects) for up to 1 h exposure;
- ERPG(2) =  $10 \text{ mg m}^{-3}$  (without serious, adverse effects) for up to 1 h exposure;
- ERPG(3) =  $30 \text{ mg m}^{-3}$  (not life threatening) up to 1 h exposure.
- Workplace Environmental Exposure Level (WEEL) [17]:
  - 8 h Time-Weighted Average (TWA) = 0.3 ppm.

According to the Indiana Relative Chemical Hazard Ranking System (IRCH, formerly known as 3P2M) [18], developed by the Indiana Clean Manufacturing Technology and Safe Materials Institute (CMTI) at Purdue University,  $\text{HSO}_3\text{Cl}$  is ranked at number 443 in respect of its toxicity in a total of more than 900 hazardous materials.

All the field tests that have been conducted were to examine the effectiveness of different mitigation treatments on  $\text{HSO}_3\text{Cl}$  spills. In 1978 and 1980, the Mond Division of ICI in collaboration with several other companies carried out a series of spillage trials at Porton Down in Wiltshire, UK [19]. Different control agents were tested on five acids. Addition of high molecular weight polyacrylamide and polymethyl methacrylate was shown to be an effective technique in suppressing fumes from  $\text{HSO}_3\text{Cl}$  and 20% oleum.

In another study, the performance of aqueous foams on selected materials was examined [20]. Hazmat NF2, a speciality foam for use on acetic materials, effectively mitigated the reactivity of 35 and 65% oleums and  $\text{TiCl}_4$  and suppressed the resulting clouds. However, this foam was not effective on  $\text{SO}_3$  and  $\text{HSO}_3\text{Cl}$  spills.

In 1990, the Ansul Company tested its product 'Spill-X-A' (magnesium oxide blended with other chemical additives) on mitigating spills of  $\text{SO}_3$ , 65% oleum and  $\text{HSO}_3\text{Cl}$  [21]. Three tests that involved spillages of  $\text{HSO}_3\text{Cl}$  were carried out. In each test, 55 gal were spilled into a 50 square foot ( $4.6 \text{ m}^2$ ) test pan. The generated pool was 1.75 in (4.1 cm) deep. The choice of a confined spill (rather than onto flat ground) was made because this would be a more severe test of the effectiveness of Spill-X-A agent. In their test report summary, it is stated that some previous testing on small (1–5 gal) flat-ground spills showed that application of Spill-X-A is an effective way of mitigating and neutralising acid vapour releases in a one-step process. It was found that application of Spill-X-A agent along with an intermittent water fog spray proved to be a fast and effective means of dealing with spills of these acids. It was most effective on  $\text{HSO}_3\text{Cl}$ , followed by 65% oleum and then sulphur trioxide as shown in Table 2.

The reaction efficiency was taken as the percentage ratio of the mass of reacted acid to the mass of acid spilled. Visual examination during the tests showed a large reduction in the fuming 5 min after the Spill-X-A agent application began. Complete control, where no potential for fuming existed, was accomplished in 10–20 min.

In the summary of this test report it is stated that reaction coefficients and control times would be better for flat-ground spills normally encountered during an accidental release.

Table 2  
Ansul test results report [21]

Acid tested	Reaction efficiency range (%)
$\text{HSO}_3\text{Cl}$	78–86
65% oleum	44–63
$\text{SO}_3$	38–54

Table 3  
DuPont spill test results [22]

	Average temperature before control (K)	Maximum temperature before control (K)	Control time (s)
Water spray	377	417.6	125
Foam	356.4	382	140
Spill-X-A	418	503	357

The advantage of this technique is that it mitigates and neutralises in one step leaving a non-hazardous RCRA (Resource Conservation and Recovery Act) waste to dispose of after clean up is complete.

The Du Pont Specialty Chemicals Company carried out field tests on mitigation methods for small spills of  $\text{HSO}_3\text{Cl}$  and oleum at the liquefied gaseous fuels spill test facility in Nevada, USA, during April and May 1992 [22]. Sixteen different tests were conducted by spilling about 25 US gal of  $\text{HSO}_3\text{Cl}$ . Three different control agents were tested: water spray, two new types of foam and Spill-X-A agent. The pan was 1.5 in deep. The results of these tests are summarised in Table 3 (it should be noted that the average temperature before control is not the starting temperature).

It should be noted that the control time was taken as the time from the start of the mitigation to the point in which fuming has essentially stopped. The following conclusions were drawn from these mitigation tests:

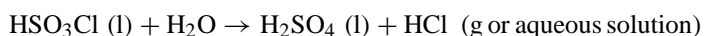
- High temperatures may result from the mitigation/neutralisation of these substances.
- Both types of foam and water spray were very effective on  $\text{HSO}_3\text{Cl}$  (control time was about the same).
- The maximum temperatures for foam mitigation tests were lower than for water mitigation tests.
- A foam blanket could not be formed until the whole amount of  $\text{HSO}_3\text{Cl}$  had reacted. This was attributed to the  $\text{HCl}$  vapour that was continuously destroying the foam blanket.
- Mitigation with Spill-X-A agent resulted in higher temperatures and longer control times. This technique was reported to be probably best suited for small spills spread out over a larger area.

The generated plume had the appearance of an opaque white cloud even though the prevailing relative humidity was quite low (about 15%). The heat of reaction of  $\text{HSO}_3\text{Cl}$  with the applied mitigating agent resulted in temperature rises above the initial temperature in the pan of up to 110 K.

These field tests further demonstrated that the reaction between  $\text{HSO}_3\text{Cl}$  and water is extremely violent and application of the control agent should be made with all the necessary precautions by an experienced person wearing protective equipment. The application of water spray and foam produced a hot non-fuming solution of  $\text{H}_2\text{SO}_4$  at the end of the mitigation procedure. This solution should be neutralised before disposal. Different substances like lime, soda ash, pot ash, limestone and Spill-X-A could be applied for this purpose. Spill-X-A neutralisation was selected in these tests because of the ease of application into the solution and also because it has been formulated to minimise the heat of reaction, and produces a non-hazardous waste.

#### 4. Reaction with water

The hydrolysis reaction with water occurs instantaneously, completely and highly exothermically in both the liquid and vapour phases. In the liquid phase, H<sub>2</sub>SO<sub>4</sub> liquid and HCl gas or aqueous solution will be formed. HCl will enter into solution only when excess water is present. Usually, this occurs when there is high availability of water (e.g. on a wet substrate or by application of water spray or aqueous foams onto the pool). In other cases, there is not enough water available and HCl will be generated in the gas phase. Overall, the hydrolysis reaction can be represented by the following equation:



In cases of HCl gas generation the heat of reaction was calculated to be equal to about  $-1115 \text{ kJ kg}^{-1}$  of water. When HCl is produced as an aqueous solution, the heat of reaction is much higher (due to the high energy of solution involved) and depends on the degree of solvation.

In the vapour phase, hydrolysis proceeds according to reaction (1). HSO<sub>3</sub>Cl vapour reacts with atmospheric moisture yielding H<sub>2</sub>SO<sub>4</sub> vapour and HCl gas. Mackay [23] has studied infrared emission from an exothermic reaction between a liquid aerosol and a gas. Significant levels of radiation were observed from the reaction of HSO<sub>3</sub>Cl aerosol with gaseous ammonia and water. Experiments have been conducted in a closed reaction tube. Some observations were made on the reaction of HSO<sub>3</sub>Cl aerosol with water but it was recommended that further investigation should be conducted before drawing conclusions.

The evaporation of HSO<sub>3</sub>Cl droplets at different moisture contents of the surrounding vapour–gas phase was studied experimentally by Nuzhnyi et al. [24]. It was shown that evaporation of a HSO<sub>3</sub>Cl droplet stops after a certain period of time, and from this point on it grows by vapour condensation. The evaporation rate and droplet temperature increase with increasing relative humidity.

#### 5. Pool behaviour and incorporation into REACTPOOL — model results

The main feature of the pool of HSO<sub>3</sub>Cl is the exothermic reaction with water. In many cases reaction with water will proceed under HSO<sub>3</sub>Cl excess conditions with HCl gas directly produced and evolved to the atmosphere, since there would not usually be much water available for HCl to enter into solution. H<sub>2</sub>SO<sub>4</sub> liquid will also be formed.

During the spreading period water is supplied to the pool from three sources: free ground water, substrate water and atmospheric moisture. In the after-spreading period water will be supplied only from the substrate and the atmosphere.

Apart from HCl, HSO<sub>3</sub>Cl will also evolve to the atmosphere in view of its high volatility. The energy produced by the reaction with water increases the pool temperature and the vapour evolution rate. H<sub>2</sub>SO<sub>4</sub> vapour may also evolve in cases where the pool temperature is quite high ( $>333 \text{ K}$ ; at these temperatures H<sub>2</sub>SO<sub>4</sub> vapour pressure becomes significant).

The pool behaviour of HSO<sub>3</sub>Cl is quite different compared to other water reactive chemicals. Specifically, two different regimes are encountered based on the amount of free ground

water available for reaction.  $\text{HSO}_3\text{Cl}$  is one of very few water reactive chemicals that reacts with water on a 1:1 molar basis. This means that excess water scenarios could be encountered more readily and in these cases water will also be present in the pool, affecting its properties.

In all cases, the pool will contain two liquids and may boil or evaporate depending on the amount of water available for reaction, and other characteristics. There is no possibility of solidification. When water is not in excess,  $\text{HSO}_3\text{Cl}$  and  $\text{H}_2\text{SO}_4$  will be present in the pool, and its properties will continuously change. In cases of excess water,  $\text{H}_2\text{SO}_4$  and water will be present, since all the available  $\text{HSO}_3\text{Cl}$  will be reacted; the pool properties will continuously change.  $\text{H}_2\text{SO}_4$  liquid will also interact with concrete surfaces as for accidental spills of  $\text{SO}_3$  and oleum [4].

The pool behaviour of  $\text{HSO}_3\text{Cl}$  has been incorporated into REACTPOOL [5]. As noted in [5], the model allows for the reaction products to be evolved in the gas phase or to be incorporated as an aqueous solution when there is excess water. However, in the case of  $\text{HSO}_3\text{Cl}$ , it has been assumed that  $\text{HCl}$  is generated in its gaseous form, although with excess water it is actually more likely that  $\text{HCl}$  will enter into solution. This assumption is necessary in this case because it is extremely difficult to calculate the degree of solvation and thence the heat of reaction and the pool properties. It might be expected that the above assumption would result in overestimation of the  $\text{HCl}$  evolution rate. It should be noted though, that if aqueous  $\text{HCl}$  is formed, the heat of reaction is much greater, and so the pool temperature is much higher compared to the case where  $\text{HCl}$  is directly generated in its gas phase. Therefore, the amount of  $\text{HCl}$  evolved may not differ greatly between these cases.

All the properties of reactants and products involved have been parameterised as functions of temperatures and are listed in Appendix A.

Critical aspects of the pool behaviour of  $\text{HSO}_3\text{Cl}$  have been revealed using REACTPOOL. Overall, the pool behaviour is strongly affected by the amount of water available for reaction. The main water source is usually the free ground water. The surface roughness and the wind speed also have a strong effect on the results. The rest of the input parameters have a weaker effect.  $\text{HSO}_3\text{Cl}$  pools usually boil in the early stages of the spreading period. For the rest of the release duration they evaporate.

In cases of high ground water availability ( $w_g \geq 0.003$  m in the scenarios investigated here), all the available  $\text{HSO}_3\text{Cl}$  is used up in the reaction with water. In these cases the pool will contain  $\text{H}_2\text{SO}_4$  liquid and excess water, its temperature will be quite high and the generated cloud will contain  $\text{HCl}$  gas and  $\text{H}_2\text{SO}_4$  vapour. Changes in the value of  $w_g$  do not have a significant effect on the amount of vapour evolved since the amount of the reaction energy supplied to the pool remains constant. However, the amount of excess water does affect the rest of the pool properties. It should be noted that in these cases, release to the atmosphere ceases just after spreading stops (Fig. 1,  $w_g = 0.003$  and  $0.005$  m). This occurs because the pool will contain only aqueous  $\text{H}_2\text{SO}_4$  liquid and its temperature in the after-spreading regime will not be high enough to allow significant evolution of  $\text{H}_2\text{SO}_4$  vapour (no free ground water is available in the after-spreading regime).

A large number of different release scenarios was examined. The values of the release scenario input parameters are shown in Table 4. The effects of significant parameters on the pool characteristics are described in Part III of this series of papers where a comparison with the pool behaviour of other water reactive chemicals is also presented [7].

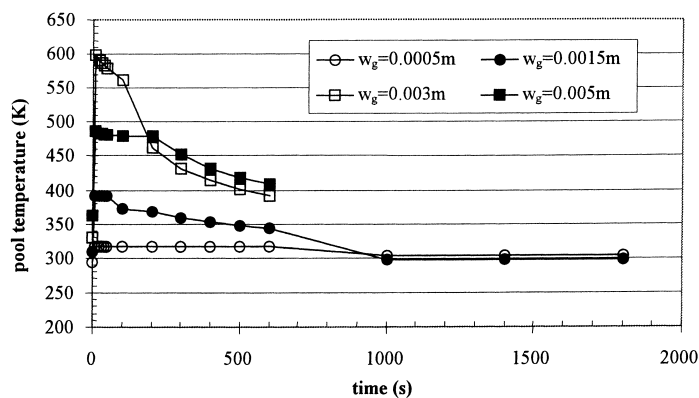


Fig. 1. Pool temperature profiles for different values of  $w_g$  ( $z_o = 0.1\text{ m}$ ,  $U_{10} = 5\text{ m s}^{-1}$ ).

Table 4

Values of the release scenario input parameters

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Spill rate and duration =  $16\text{ kg s}^{-1}$  for 600 s  
 Maximum duration of release to the atmosphere = 1800 s  
 Maximum pool radius = 50 m  
 Type of substrate = concrete  
 Free water film thickness on the ground,  $w_g = 0.0005, 0.0015, 0.003,$  and  $0.005\text{ m}$   
 Surface roughness length,  $z_o = 0.1, 0.01, 0.001,$  and  $0.0001\text{ m}$  ( $h_{\min} = 1\text{ cm}, 8.5,$   
 $7$  and  $5\text{ mm}$ , respectively)  
 Wind speed at 10 m,  $U_{10} = 5, 2,$  and  $10\text{ m s}^{-1}$   
 Air temperature = Release temperature = 288 K  
 Atmospheric radiation factor = 0.84  
 Cloud cover factor = 7  
 Relative humidity = 70%  
 Location = North England, UK (latitude =  $54^\circ$ , longitude =  $2^\circ$ )  
 Time and day = 09 : 00 h and 298 (25 October)  
 Time step used in the calculations = 0.01 s

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Figs. 1–6 show the results for the above scenarios. These show the behaviour of the main pool properties and vapour evolution rates. The detailed commentary on these results is given in the comparative discussion in Part III of this series of papers [7].

## 6. Behaviour of the generated cloud

Clouds generated from accidental spills of  $\text{HSO}_3\text{Cl}$  will initially contain  $\text{HSO}_3\text{Cl}$  vapour,  $\text{HCl}$  gas and possibly some small amounts of  $\text{H}_2\text{SO}_4$  vapour, in cases where the water supply in the pool is not in excess. Under excess water conditions, the generated cloud will initially contain  $\text{HCl}$  gas and  $\text{H}_2\text{SO}_4$  vapour.

The cloud behaviour will resemble in many respects the behaviour of a  $\text{SO}_3/\text{oleum}$  cloud [25], with the additional complexity of a third component, namely  $\text{HCl}$ .



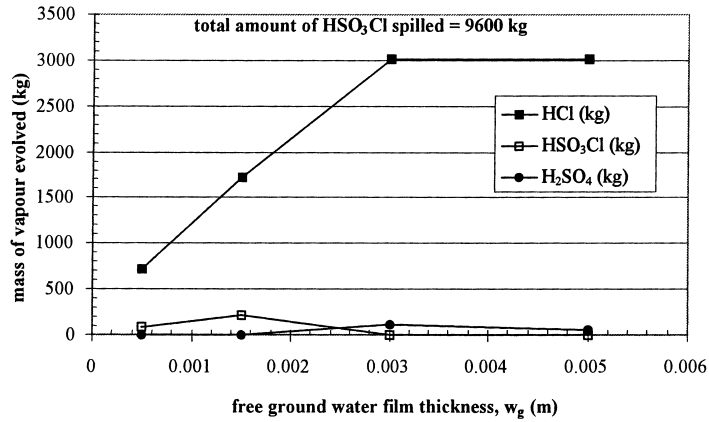


Fig. 2. Effect of  $w_g$  on the total amount of vapour evolved for the total release duration ( $t_{s2} = 1800$  s) ( $z_o = 0.1$  m,  $U_{10} = 5$  m s<sup>-1</sup>).

## 7. Discussion, conclusions, further investigation

Chlorosulphonic acid is a toxic material that can severely harm humans and the environment. When accidentally spilled it creates a liquid pool, the main feature of which is the exothermic reaction with water.

In respect of its toxicity very limited data are available. More investigation is required in this field in order to draw firmer conclusions.

The literature revealed no published attempts to model the pool or cloud behaviour. An extensive survey of any relevant information sources was conducted in the course of

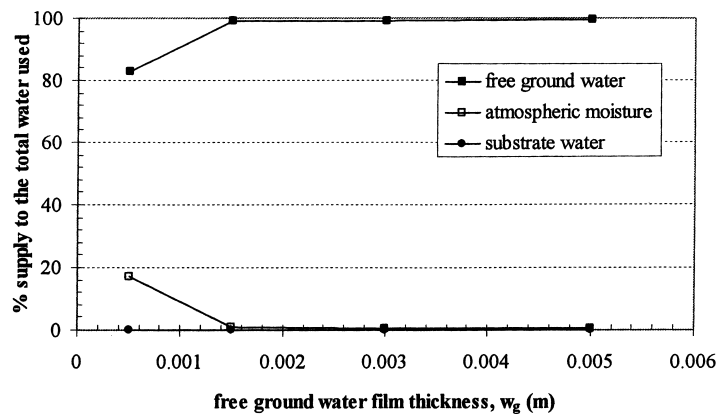


Fig. 3. Percentage supply of the three water sources to the total amount of water provided for reaction with HSO<sub>3</sub>Cl for spills of 16 kg s<sup>-1</sup> for 600 s ( $z_o = 0.1$  m,  $U_{10} = 5$  m s<sup>-1</sup>).

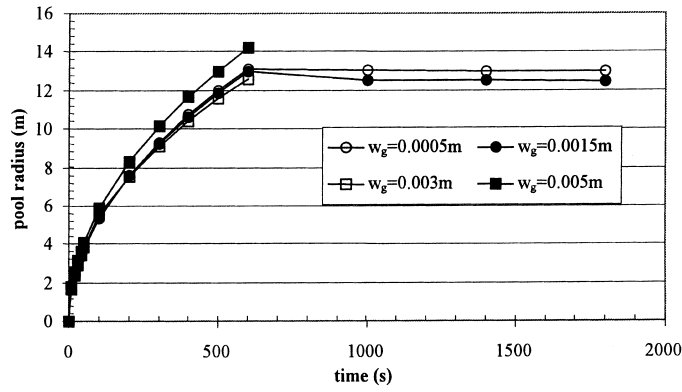


Fig. 4. Pool radius profiles for different values of  $w_g$  ( $z_o = 0.1$  m,  $U_{10} = 5$  m s<sup>-1</sup>).

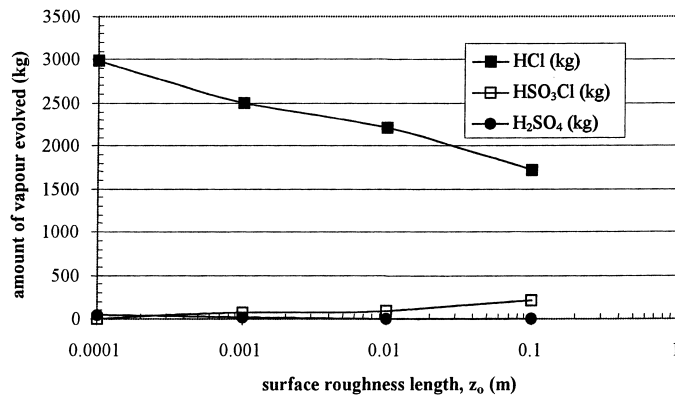


Fig. 5. Effect of  $z_o$  on the total amount of vapour evolved for the total release duration ( $t_{s2} = 1800$  s) ( $w_g = 0.0015$  m,  $U_{10} = 5$  m s<sup>-1</sup>).

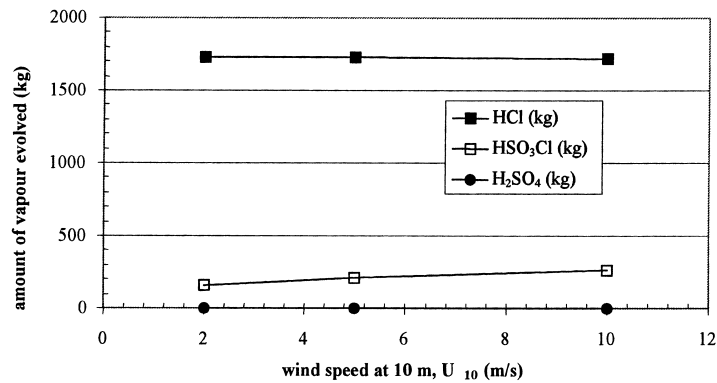


Fig. 6. Effect of  $U_{10}$  on the total amount of vapour evolved for the total release duration ( $t_{s2} = 1800$  s) ( $w_g = 0.0015$  m,  $z_o = 0.1$  m).

this study. A number of different release scenarios were investigated using REACTPOOL, the use of which gave useful insights into the behaviour of such spills. It is very easy to use and calculation times were very satisfactory. Although  $\text{HSO}_3\text{Cl}$  has been involved in major accidents, no experiments have been conducted to test its release behaviour. Further improvement and validation of the model depends on the availability of these data.

Further investigation will be focused on describing and modelling the behaviour of the generated cloud created from accidental spills of  $\text{H}_2\text{SO}_3\text{Cl}$ . The behaviour of such a cloud resembles the behaviour of clouds generated from  $\text{SO}_3$  and oleum spills.

## Acknowledgements

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## Appendix A

Various sources were used to identify the properties of  $\text{HSO}_3\text{Cl}$  and  $\text{H}_2\text{SO}_4$  [8–11,26]. In this paper, only the properties of  $\text{HSO}_3\text{Cl}$  are reported. The properties of  $\text{H}_2\text{SO}_4$  are readily available in most chemical handbooks.

### A.1. Properties of liquid $\text{HSO}_3\text{Cl}$

Molecular weight, MW	116.525 g mol <sup>-1</sup>
Boiling point, bp	428 K
Freezing point, fp	193 K
Liquid density, $\rho$ (kg m <sup>-3</sup> ) ( $T$ (K))	$\rho = 596.72 \times 0.2852^{(-1-T/700)^{0.28571}}$
Heat capacity, $C_p$ (kJ kg <sup>-1</sup> K <sup>-1</sup> )	$C_p = 1.204 + 1.402 \times 10^{-4} T - 2.887 \times 10^{-6} T^2$
Viscosity, $\mu$ (cP)	$\log \mu = -0.5472 + (126.93/T) + 1.0574 \times 10^{-3} T - 3.6166 \times 10^{-6} T^2$
Thermal conductivity, $k$ (kW m <sup>-1</sup> K <sup>-1</sup> )	$k = 0.208 \times 10^{-3} - 1.1086 \times 10^{-7} T - 1.6832 \times 10^{-10} T^2$
Vapour pressure, $P$ (mmHg)	$\log P = -5.604 - (2760.4/T) + 8.4466 \log T - 2.2029 \times 10^{-2} T + 1.1699 \times 10^{-5} T^2$
Heat of vapourisation, $H$ (kJ kg <sup>-1</sup> )	$H = 528.3(1 - T/700)^{0.443}$
Schmidt number, $Sc$ (estimated according to reference [26])	1.64
Critical temperature, $T_c$ (K)	700
Critical volume, $V_c$ (cm <sup>3</sup> mol <sup>-1</sup> )	195

## References

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