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Comparison of results from some chemical dispersion models and hazard prediction and assessment tools

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English summary

Dispersion models and hazard prediction and assessment software tools are used to assess consequences from dispersion of hazardous materials, such as toxic chemicals. Such tools can be employed during and after an event to support crisis and consequence management, or to assess hypothetical scenarios for emergency preparedness planning, training and exercises. The software HPAC, ARGOS, DEGADIS, NBC-Analysis, ERGO and “Farlig gods” are compared by performing calculations of the dispersions and predicted hazard areas for the three scenarios: rupture of a tank containing 20 tonnes of pressurized liquefied chlorine, rupture of a tank containing 10 tonnes of pressurized liquefied ammonia, and finally an attack with soman by bomber aircrafts. For the first two scenarios, several meteorological conditions are considered.

The motivations of this study are: to investigate the required input parameters and exemplify possible output of the various tools; to outline the assumptions and limitations of the programs; and to discuss the user friendliness and the pre-required user knowledge and competence.

The main conclusions are:

- The box model for heavy gases (DEGADIS) and the Gaussian dispersion models which are included in two decision support systems (HPAC and ARGOS) give large variations in calculated plume prediction patterns for the three scenarios. Not all programs are suited for all scenarios. Hence, decisions based solely on the use of one of these programs can lead to serious misjudgements. It is important to have several models available and to know which model to employ for a given scenario. FFI will continue to test and evaluate these and possible other models for other scenarios.
- A fairly high user competence level is required for HPAC, ARGOS and DEGADIS.
- When HPAC or ARGOS is used in an operation or in a crisis situation, a real-time connection to a meteorological service is highly desirable.
- The “Farlig gods” program and ERGO are both simple to use, even for inexperienced users. They only give areas where protective actions should be considered. NBC-Analysis gives no safety distances based on quantitative hazard levels, but produces an area which is considered unsafe to enter.
- The inter-comparison of results in this study is purely based on a relative comparison since the true dispersion patterns for selected scenarios are not known. There is an urgent need for additional experimental data in order to have data sets for model validation and improvements. FFI is currently pursuing this goal through international collaborations and project initiatives.

Sammendrag

Spredningsmodeller og fareprediksjonsverktøy blir brukt til å vurdere konsekvenser fra spredning av helseskadelige materialer slik som giftige kjemikalier. Slike verktøy kan benyttes under og etter en hendelse for å støtte krisehåndteringen, eller for å analysere hypotetiske scenarioer for bruk til beredskapsplanlegging, trening og øvelser. Programvarene HPAC, ARGOS, DEGADIS, NBC Analysis, ERGO og ”Farlig gods” er sammenlignet ved å utføre spredningsberegninger og fareprediksjon for følgende tre scenarioer: revnet tankbil med 20 tonn trykksatt væskeformig klor, revnet tank med 10 tonn trykksatt væskeformig ammoniakk, og et bombeangrep med det kjemiske stridsmiddelet soman. I de to første scenarioene ble flere ulike meteorologiske betingelser testet.

Motivasjonen for studien er: å undersøke hva som er nødvendige inngangsverdier, samt å eksemplifisere mulige resultater ved bruk av de ulike programmene; å skissere antakelsene og begrensningene for programpakkene; og å diskutere brukervennlighet og nødvendig kunnskap og kompetanse for brukerne.

De viktigste konklusjonene er:

- Boksmodellen for tunge gasser (DEGADIS) og de gaussiske spredningsmodellene i beslutningsstøtteverktøyene (HPAC og ARGOS) gir store variasjoner i beregnet spredningsforløp for de tre scenarioene. Ikke alle programmer er egnet for alle scenarioer. Beslutninger basert kun på bruk av ett av disse programmene kan derfor føre til alvorlige feilvurderinger. Det er viktig å ha flere modeller tilgjengelig og vite hvilken modell som bør brukes for et gitt scenario. FFI vil fortsette å evaluere disse og andre mulige modeller for andre scenarioer.
- HPAC, ARGOS og DEGADIS krever et relativt høyt kompetansenivå hos brukeren.
- Når HPAC og ARGOS brukes operasjonelt i en krisesituasjon, er det sterkt ønskelig med en direkte kobling i sanntid til en værtjeneste slik at meteorologiske data i det riktige formatet kan lastes inn.
- Programmene “Farlig gods” og ERGO er begge enkle å bruke, også for uerfarne brukere. De gir kun sikkerhetsavstander der beskyttelsestiltak bør vurderes. NBC-Analysis gir ikke sikkerhetsavstander basert på kvantitative farenivåer, men angir et område som vurderes som risikabelt.
- Resultatene i denne studien er kun basert på relative sammenlikninger siden den sanne spredningen av gasser i de valgte scenarioene ikke er kjent. Det er et presserende behov for flere eksperimentelle data for å bli i stand til å validere og forbedre de tilgjengelige modellene. FFI er i ferd med å gjennomføre dette gjennom internasjonale samarbeidsprosjekter.

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Preface

The authors would like to thank Jan Henrik Blanch for his valuable comments and for his comparison of our results with the results from his own prediction program WinVap. We would also like to thank the people at Prolog Development Center and Risø National Laboratory for their excellent assistance when we had questions regarding ARGOS. Thanks also to Jan Steen Jensen at the Danish Emergency Management Agency, Jan Erik Dyve at the Norwegian Radiation Protection Authority and Paul Taylor at Bruhn NewTech for reading the manuscript and suggesting valuable corrections and improvements.

1 Introduction

Upon aerial dispersion of hazardous chemicals or other hazardous material which causes an acute military or civilian crisis situation, there will be an urgent need to identify and predict the plume transport pattern (speed, direction and concentrations) in order to:

- Warn personnel and the general public
- Aid decisions regarding evacuation
- Support rescue operations
- Support decisions on needs for protective equipment and detection devices
- Define the area for hazard monitoring and sampling

Atmospheric dispersion models and hazard prediction and assessment software tools are used for this purpose, i.e. to assess consequences from dispersion of hazardous materials such as toxic chemicals and/or radioactive particles. Such tools are employed during and after an event to support crisis and consequence management. Another important application is to assess hypothetical scenarios for use in emergency preparedness planning, training and exercises, and to identify needed protection factors for equipment and detectors.

The complexity of atmospheric dispersion models varies depending on the modelling assumptions and simplifications, and thus also their computational costs. FFI uses both complex Computational Fluid Dynamics (CFD) and faster dispersion models, and hazard assessments tools. The focus of the present work is a comparison of available operational response systems which can assist decision making during the initial phase of an acute crisis. Although available computational resources are steadily increasing, the computational costs of CFD modelling currently limit this approach to preparatory and post-incident applications.

Since crucial decisions are made based on models and tools, it is important that the predictions can be trusted to be as close to reality as possible. Erroneous predictions, both underpredictions and overpredictions, can have serious consequences. Underpredictions may delay operations to protect personnel and the public thus putting lives and health at immediate risk. Overpredictions may cause unnecessary intrusive measures, such as evacuating too many, or deny access to areas or key resources. To ensure a sound interpretation of hazard predictions, users must know the limitations and shortfalls of models and tools. Models must be validated against measured data for relevant incidents and against controlled experimental data in order to give the users the a priori needed information. Since such experiments are complex to set up and very costly, there is a general lack of such data for model validation and comparison.

In a recent project under the European Defence Agency (EDA), some fast hazard assessment tools and Gaussian dispersion models were used to analyse possible consequences of chlorine release from a tanker truck [1]. The results showed large variations which we need to better understand. The motivation of the present study is to enhance our understanding of these programs by more systematically comparing and possibly explaining varying result, and to document user experience and important underlying assumptions and limitations of these program packages.

Specifically, the objectives of the present study are:

- To calculate aerial dispersion and predict hazard areas using one box model for heavy gases (DEGADIS) and the Gaussian dispersion models which are included in two decision support systems (HPAC and ARGOS).
- To compare hazard prediction and assessment tools (NBC-Analysis, ERGO and "Farlig gods").
- To illustrate what type of user input parameters the selected models and tools require.
- To illustrate what type of output and information the models and tools provide to the user.
- To outline the main underlying assumptions and purposes of the models that users should be aware of.
- To discuss the user friendliness and required user knowledge and competence.

The objectives will be achieved by utilizing three hypothetical scenarios involving dispersion of toxic chemicals; a chemical warfare agent (soman) and two toxic industrial chemicals (chlorine and ammonia). It is important to note that there are no experimental data available for the selected scenarios, thus the true dispersion patterns are unknown. Hence, an inter-comparison of model results for these scenarios is purely relative.[1]

In this study we have considered software packages used by the Norwegian Defence and FFI. NBC-Analysis and ERGO are the tools currently used by the Norwegian Armed Forces. HPAC, which is a program package used by the U.S. and many NATO countries, is also included. It is used in NATO studies and by NATO groups. FFI has applied it for various scenario assessments used in previous studies and exercises. ARGOS is the dispersion model implemented by the Norwegian Radiation Protection Authority (NRPA) as well as by several other radiation protection authorities worldwide. Norway participates in the ARGOS consortium through NRPA. ARGOS is primarily developed for hazard predictions for radiological incidents, but a chemical module has recently been added. FFI wanted to explore ARGOS for possible future use. DEGADIS is a dense gas dispersion model developed for the U.S. Environmental Protection Authority (EPA). FFI has used DEGADIS previously when studying the dispersion of dense gas (chlorine). "Farlig gods" is a computerised version of the Norwegian hazard assessment guidelines issued by the Directorate for Civil Protection and Emergency Planning (DSB). "Farlig gods" is used by first responders in Norway.

We have selected three different scenarios in this study, starting from the simplest case and moving towards more complicated cases. This has been done because we wanted to investigate the effect of the different input parameters in the simulations, and also because this work was a

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[1] There is an urgent need for well-defined experimental measurements of dispersion of toxic chemicals in various types of topographies which can be employed in dispersion model development, inter-comparison and validation.

process by which we learned how to use the programs. A description of the scenarios used in this study is given in Table 1.1:

Scenario	Location	Toxic chemical	Focus of comparison
1a	Ørland	Chlorine	Different terrain (land and sea)
1b	Ørland	Chlorine	Meteorological data from two heights
1c	Ørland	Chlorine	Source term modelling included
2	Kjeller	Ammonia	Season variations (different meteorological conditions: winter, summer, autumn)
3	Bodø	Soman	Attack from three enemy aircrafts (two different bomb loads)

Table 1.1 Scenarios used in this report.

The work presented in this report is part of FFI's research efforts since 2003 for the Norwegian Defence Forces in dispersion modelling and hazard prediction (FFI projects 859, 1048 and now 1149). The long term objective is for FFI to be expert users in dispersion models and hazard assessment tools that are relevant to the Norwegian Defence, to cover the spectrum of need, and to contribute to improve these packages both through experiments and numerical simulations. In this context FFI has participated in the European Defence Agency (EDA) project "NBC modelling and simulation", and has an ongoing and valuable collaboration with the U.S. Naval Surface Warfare Center on release and dispersion of dense gases which includes participation in field experiments financed by the U.S. Department of Homeland Security. FFI is currently taking an initiative to launch an EDA project on urban dispersion of dense gases which includes high fidelity numerical simulations and experiments with the objective to establish a much needed database of experimental data for model development and improvement and to have sufficient data to quantify the performance of operational models.

The structure of the report is as follows: Chapter 2 contains general information about the dispersion models and hazard assessment software used in this study and a short introduction to meteorological stability classes and surface roughness parameters. Chapter 3 discusses source modelling. Chapters 4-6 present the dispersion modelling and simulation results for each of the hypothetical scenarios with chlorine, ammonia and soman. Results from each model are presented and discussed. Chapter 7 discusses user experiences for the various software packages. Chapter 8 presents conclusions from this study.

2 Background

2.1 Operational response systems

The present work presents the use of two types of operational response systems for decision support upon release of hazardous chemicals:

- Hazard prediction and assessment tools
- Atmospheric dispersion models

Hazard prediction and assessment tools provide operational advice on the potential size of hazardous areas. No actual atmospheric dispersion modelling is performed, although the hazard distances can be based on such simulations as is the case for ERGO.

An atmospheric dispersion model includes mathematical, physical and chemical descriptions of various phenomena which combined constitute a release and dispersion incident of a hazardous compound. A dispersion model can be divided in three parts:

- Source model
- Transport model
- Effects model

The source model, or release characteristics, describes the release of the hazardous compound into the atmosphere based on its physical and chemical properties, release location, amount and the mechanism of release.

The transport model describes atmospheric transport of the hazardous compound from the release location and the downwind concentrations. This process depends on the three-dimensional wind field, its time variations and interactions with the hazardous compound. Important atmospheric input parameters are wind speed and direction, temperature, and the atmospheric stability.

The effects model describes how the concentrations of the hazardous compound affect human health and the environment. Human health effects depend on the toxicological properties of the hazardous compound for the relevant concentrations, exposure routes and exposure durations and the susceptibility of the exposed individuals. This has not been dealt with in this report.

The wind field can in principle be described by a set of partial differential equations called the Navier-Stokes equations, which are derived from the fundamental physical principles of conservation of mass, momentum and energy. There is no exact analytical solution for these equations, thus one must either simplify the wind field description, or solve these equations numerically at high computational costs. In addition, non-linearities in the Navier-Stokes equations manifest themselves as turbulence, a chaotic mixing process involving energy transfer between large and small scales which enhances dispersion. All turbulent scales cannot be represented even using the most powerful computers available, hence turbulence must be modelled. In Computational Fluid Dynamics (CFD), the Navier-Stokes equations are replaced by equations describing the statistical properties, and these are solved numerically.

The hazardous compounds may be transported in a gaseous state or as liquid or solid particles suspended in air (aerosols). Gaseous dispersion can be described by a transport equation including advection (transport by the wind field) and dispersion due to molecular and turbulent diffusion. If the contaminant density differs from the air density, this must be taken into account since the wind field will be affected. In particular, will gravity effects be important for dense gas dispersion. Neutral gases or low contaminant concentrations can, on the other, hand be treated as a passive dispersion which does not affect the wind field. Particulate releases can either be approximated by an advection/diffusion equation or described by discrete particle models. Particles are influenced by numerous forces, e.g. gravity and frictional forces. Hence, two crucial parts of atmospheric dispersion modelling are:

- The wind field description, including the effects of turbulence
- The model for dispersion of the hazardous compound

Atmospheric dispersion models are often categorized based on their complexity, simplifications in wind field descriptions and application areas. Gjesdal gives a short overview of models for dispersion simulation and a simple classification of models is reproduced in Table 2.1[2]. For a more detailed introduction to dispersion models for emergency management we also refer to ref [3].

Scale		**Model**
Near-field	0 – 2000 m	Computational Fluid Dynamics (CFD)
Local	100 m – 10 km	Gaussian dispersion models Box models
Long distance	>10 km	Particle models

Table 2.1 Simplified classification of dispersion models.

Simplified models usually assume that the wind field is constant in direction and speed. This assumption may only be valid for open terrain and are usually only applicable for passive dispersion, i.e. when the density of the contaminant is similar to air or the concentrations are low. The dispersion model can be represented by Gaussian distribution functions, and such models are referred to as Gaussian dispersion models. Model parameters are determined based on the surface characteristics and meteorological conditions. Such models can be applied for both continuous and instantaneous releases. Models for instantaneous emissions are referred to as Gaussian puff models. Under the above assumptions, Gaussian puff models can give good estimates on the scale 100 m -10 km.

Dispersion of dense gasses behaves differently than passive dispersion. Gravity effects cause increased horizontal spreading and reduced plume height. Density differences also affect the motion of the air substantially, and thereby also the mixing process. These effects have been demonstrated in field experiments [4]. Special models, so called box models, have been developed for dense gas dispersion. These correspond to Gaussian models in complexity and represent a gas plume which collapses under gravity.

The simplified Gaussian and box models are developed for cases where the wind field is known and relatively constant. These assumptions are not valid for releases in complex geometries, i.e. near buildings and large topographical variations, since wind and turbulence is greatly affected. Near the release point it is necessary to calculate the wind field including turbulence using CFD models, which are best suited in the region 0 – 2000 m.

Due to wind field variations it is necessary to include meteorology models for dispersion of hazardous compounds on distances longer than 10 km. The dispersion model is typically a particle model in which particles or Gaussian puffs are advected by the wind field.

The objective of the present work is to compare some operational response systems used by the Norwegian Defence and at FFI which can assist decision making during an intentional or unintentional release of toxic chemicals. CFD models are not included since the computational time is too long. The operational response systems used in this study are presented in the next chapters. The hazard prediction and assessment tools ERGO and “Farlig gods” are described in Chapter 2.2; NBC Analysis is described in Chapter 2.3; and the software packages HPAC, ARGOS based on Gaussian dispersion models, and the box model DEGADIS are presented in Chapter 2.4.

In the present work, we focus primarily on comparison of the transport modelling of the selected dispersion modelling software. Hence, we have used the same release descriptions, meteorological input parameters and the same threshold values for toxicological effects.

2.2 Hazard prediction and assessment tools

2.2.1 Emergency Response Guidebook (ERGO)

The Emergency Response Guidebook was developed jointly by Transport Canada (TC), the U.S. Department of Transportation (DOT), the Secretariat of Transport and Communications of Mexico (SCT) and with the collaboration of CIQUIME (Centro de Información Química para Emergencias) of Argentina [5]. CANUTEC's ERGO 2008 is a software version of ERG2008 and can be downloaded free of charge from the CANUTEC website. It has been developed for fire fighters, police, and other emergency services personnel. It is primarily a guide to aid first responders to quickly identify the specific or generic hazards of hazardous materials involved in an incident, and protecting personnel and the general public during the initial response phase. In this phase the presence and/or identification of dangerous goods is confirmed, protective actions and area cordons are established, and assistance from qualified personnel is requested. It is not intended to provide information on the physical or chemical properties of dangerous goods.

ERG2008 is primarily designed for use at a dangerous goods incident occurring on a highway or railroad. Application at fixed facility locations may be of limited value. ERGO 2008 incorporates dangerous goods lists from the most recent United Nations (UN) recommendations as well as from other international and national regulations.

ERG2008 gives Initial Isolation and Protective Action Distances (IIPAD) for most hazardous chemicals, in the cases of small or large spills, occurring during day or night. The IIPAD depends on several properties of the toxic industrial material (TIM) in question. It incorporates toxicity, volatility and reactivity with water. It also accounts for the container types and sizes authorised for transport. For each chemical, thousands of hypothetical releases have been modelled. The emission model calculates the release of vapour due to evaporation of pools on the ground, direct release of vapours from the container, or a combination of both. Based on statistical evaluation, the 90th percentile Protection Action Distance (PAD)[2] has been selected and listed in ERG2008.

The distances in ERGO 2008 are given for small spills (less than 200 litres for liquids and 300 kg for solids) and for large spills (greater than 200 litres for liquids and 300 kg for solids), separately. An exception to this is certain chemical warfare agents, where small spills include releases up to 2 kg and large spills include releases up to 25 kg. Different IIPADs are given for day-time and night-time releases. For more details about the IIPAD calculation, see the ERG2008 handbook [5].

2.2.2 ”Farlig gods”

The Directorate for Civil Protection and Emergency Planning (DSB) has together with the Norwegian Fire Brigade developed a handbook containing information on numerous hazardous materials stored and shipped in Norway (“Farlig gods”-permen). Based on this handbook, DSB has developed a computer program, “Farlig gods”, containing all the information of the printed version and some additional functionality [6]. The computer program contains information about hazardous materials, their properties and safety precautions. “Farlig gods” 2008 version 2.0 represents an expansion of version 1 with information on 850 hazardous materials (previously 250). Information on some chemical warfare agents has also been included in the second version. The program can be downloaded for free from the internet on DSBs homepage. The program is very user friendly and the user entry level is low.

The electronic version has, for example, search options for UN-numbers, the option to calculate recommended safety distances, and the possibility to complete required reports in case of hazardous materials incidents. The purpose of this program is to provide first responders, who are in charge of mitigating effects of a hazardous materials incident, needed and easily understandable information regarding the relevant chemical(s) in a timely and efficient manner. Based on available information first responders will be able to assess

- Possible hazards to the first responders and the general population

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[2] This means that 90% of the simulations for the statistical evaluation falls within the 90th percentile PAD.

- Possible measures which can be implemented in order to mitigate the consequences for people and the environment
- Physical and chemical properties and possible dispersion of hazardous concentrations of the chemical(s).

One of the options of the program is safety distance calculations. DSB recommends that this function is applied with caution. The method should be limited to toxic gases and large accidents (tanker trucks and rail wagons). The safety distances are guidelines only intended for the acute phase. The method is simple, and temperature is the only required input parameter. The program calculates the vapour pressure at the given temperatures, and it is assumed that the vapour pressure in kPa corresponds directly to a recommended safety distance (1 kPa = 1m). This function is used for the scenarios involving dispersion of toxic gases; i.e. chlorine and ammonia. It is not applicable, nor available, for nerve agents which are liquids at ambient conditions.

2.3 NBC-Analysis

NBC-Analysis from Bruhn NewTech is a computerised Chemical, Biological, Radiological and Nuclear (CBRN) hazard prediction, CBRN intelligence decision support and warning and reporting tool. It is designed to provide mainly military commanders with rapid and accurate information using real time reports from source level to higher commands. The program automates the CBRN calculations laid down in NATO's Warning and Reporting publications, ATP-45 [7] and AEP-45 [8]. According to Bruhn NewTech, there are over 8,000 users, and NBC-Analysis is currently in operational use in the majority of NATO and Partnership for Peace (PfP) nations [9].

The Norwegian Defence uses NBC-Analysis for CBRN hazard prediction and assessment. NBC-Analysis is installed on some stand-alone computers dedicated for use in a crisis and war. NBC-Analysis is also installed on the Norwegian Defence FIS-basis network (Classification Restricted) for training purposes. For release of toxic industrial materials, ATP-45 has adapted a hazard prediction procedure based on the Emergency Response Guidelines (ERG). These procedures are included in NBC-Analysis through the ERGO 2004 version of the ERG Guidelines. The new version (ERGO 2008) gives slightly different predictions[3]. We report results from both ERGO versions.

NBC-Analysis is capable of producing very rapid (typically less than 30 seconds) hazard warning templates on a wide variety of electronic map types. This visual template is the tool for delivering immediate hazard warnings and organizing initial response to a CBRN incident while more data on agent type and quantity, delivery means and actual (as opposed to forecast) meteorological conditions can be collected.

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[3] The coming version av NBC-Analysis (version 12), which will be called CBRN-Analysis, will use the ERGO 2008 version of the ERG Guidelines. This version will be released ultimo 2010.

A number of plume prediction models (like HPAC from DTRA and HAPPIE/RIOT from TNO) have been integrated to operate alongside the standard ATP-45 output of NBC-Analysis. In this way, the input data could be transferred directly to NBC-Analysis and the results from the plume predictions could be displayed on the same map as the NBC-Analysis results. Some of these integrated versions of the core program enable more detailed predictions of hazard downwind distances and effects to be produced. These, however, are slower, and should be used after the initial warning and evacuation actions have been completed. An advantage of separating the plume prediction models from the decision support system is that it enables flexibility in the choice of models to use.

It is possible to enter information from CBR-sensors manually into NBC-Analysis. It is also possible to import sensor information automatically. The Sensor Connectivity Integration Management solution (SCIM^{TM} solution) from Bruhn NewTech can be used to capture critical sensor alarms, convert data and transfer data to NBC-Analysis for further analysis. SCIM^{TM} provides sensor connectivity to multiple brands of sensor systems.

Version 11.0.1 of NBC- Analysis is used in this report. The attack area and hazard area are defined as follows (ATP-45(C) paragraph 1202 page 12-1 [7]):

- **Attack area** is the predicted area immediately affected by the delivered chemical agent on land. The attack area is represented by a circle in the plots from NBC-Analysis.
- **Hazard area** is the predicted area in which unprotected personnel may be affected by vapour spreading downwind from the attack area. The downwind distance of the hazard area depends on the type of attack, the weather and terrain in the attack area and the area downwind of the attack area. The shape of the hazard area depends on the wind speeds (circular for wind speeds less than 10 km/h (2.8 m/s) and a 60º sector for wind speeds greater than 10 km/h).

The predicted attack area and predicted hazard area are calculated directly after an attack or release has occurred and is reported as an NBC-3 message. Upon receipt of additional information, like a change in weather conditions, recalculations and new plots are generated and reported. After a detector survey has been conducted, and the areas of actual contamination have been defined, these areas are reported using NBC-5 and NBC-6 messages.

For toxic industrial material release from transport vehicles the procedure is adapted from the Emergency response Guidebook (ERG), (see ATP-45 (C) pages 14-6 and 14-7 [7]):

- **Release area** is assumed to be a circle with a radius equal to the isolation distance from ERGO 2004. If the UN number is not available, use a radius of 915 m.
- **Protective action distance** is given by ERGO 2004 for small spills (less than 200 litres for liquids and 300 kg for solids) and for large spills (greater than 200 litres for liquids and 300 kg for solids), separately. If the spill is greater than 1500 kg, ATP-45 states that the protective action distance should be doubled. If the UN number is not available use 11 km.

The ATP-45 procedures are currently under substantial review, and a new ratification draft ATP-45(D)-RD-1 has been issued [10]. The structure of ATP-45 has been improved, harmonized and updated in accordance with changes in NATO CBRN terms and definitions. It is easier to navigate in the document. Chemical, biological, radiological and nuclear hazard predictions and warnings have been organized in four separate chapters, and the sequence of chapters is more logical. The main difference in plotting techniques in ATP-45(D), as compared to ATP-45(C), is that plotting procedures are now divided in the following three levels for all types of attacks and releases (ATP-45(D) p 1-10):

"Simplified procedures *are those procedures intended to be manually performed by a CBRN defence staff immediately upon receipt of a message indicating a new CBRN incident. These procedures, covered within ATP-45, will be as simple as possible and deal only with the first initial message(s), without taking into consideration recalculation in accordance with upcoming weather periods.*

Detailed procedures *are those procedures intended to be performed manually or by an automated system using one or more messages. The procedures, covered within ATP-45, are only as complicated and time consuming as required for essential CBRN Warning and Reporting (W&R) capability. The output can be updated upon receipt of new information.*

Enhanced procedures *are those procedures intended to be performed only by an automated system due to complexity and/or time requirements. The output is immediately updated upon receipt of new data and is controlled by an operator. Enhanced procedures are covered within AEP-45."*

The simplified procedures will likely save time in issuing the first CBRN alert, but they are only intended for immediate warning. Another change is that all types of chemical incidents on land, i.e. chemical weapon attacks, chemical releases of unknown origin and chemical substance releases from for instance containers, are included within one Chapter (Chapter 3). The old term ROTA ("Releases other than attack") is no longer used, and NBC has been changed to CBRN throughout the document.

For TIC releases, ATP-45 (D) also adapts procedures based on ERG values, but have introduced additional spill size correction factors for extra large spills. In summary, the correction factors are (p 3-38):

- Small release – use ERG small spill values (≤ 200 L)
- Medium release – use ERG large spill values (>200 L, ≤ 1 500 Kg)
- Large release – multiply the ERG large spill values by 2 (>1 500 Kg, ≤ 50 000 Kg)
- Extra large release – multiply the ERG large spill values by 6 (> 50 000 Kg)
- Unknown size release – multiply the ERG large spill values by 2

A new version (version 12) of NBC-Analysis which incorporates the changes in ATP-45 will tentatively be ready by the end of 2010. NBC-Analysis will then change name to CBRN-Analysis.

2.4 Dispersion models

2.4.1 HPAC

Hazard Prediction and Assessment Capability (HPAC) is a package of software modules and legacy codes which predicts the dispersion from hazardous material releases and the collateral effect on the exposed population. HPAC is distributed and updated by the U.S. Defence Threat Reduction Agency (DTRA) [11]. In the program there are four basic components:

1. Source term incident models which calculate the initial characteristics of a hazardous material release based on simple inputs (where, what, when) from the user.
2. Routines and databases to provide environmental input (weather/ terrain) that can be used in the transport calculation of the hazardous material.
3. Transport calculation model that calculates how the released material disperses through the environment and determines the deposition of the hazardous materials as a function of time. The model used is the second order closure integrated puff model (SCIPUFF)[12].
4. Output module which can display the results either as footprint plots or as casualty tables based on human effect models and the exposed population after a calculation.

These components are implemented together into a graphic user interface (GUI), and it is this project editor which provides the interactive management of the HPAC projects.

2.4.1.1 Source term definition

The source term defines the release of the hazardous material. When defining the release the user can make use of one of the integrated incident models in HPAC:

- Building Interior and Exfiltration Model (BINEX)
- Chemical/Biological Facility Damage (CBFAC)
- Industrial FACilities (IFAC)
- Industrial Transportation (ITRANS)
- Urban
- Nuclear Facility Accident (NFAC)
- Chemical/Biological Weapon (CBWPN)
- Nuclear Weapon (NWPN) SE
- Nuclear Weapon Incident/Accident (NWI)
- Missile Intercept (MINT)
- Radiological Weapon Incident (RWPN)

When using one of these incident models, HPAC will translate the incident inputs (where, what and when) into a release which is used for the transport calculation of the resulting hazardous material. The resulting release can be instantaneous or continuous, stationary or moving, and is defined through a description of one or more puffs of the hazardous material released into the environment. The puff definitions will include the physical properties of the associated material and several properties such as the amount of material, the size and the location of the puff in addition to the time at which the puff release occurred. The hazardous material in the released puffs can be solid particles, liquid droplets or gaseous materials, with both primary and secondary evaporation mechanisms that produce vapour puffs as the droplets evaporate in the air or after deposition on the ground.

It is also possible to define a release directly in the project editor without using any of the incident models. This way a release can be accurately represented if the source term is well known. Such a release is called an analytical release, and to create or edit an analytical release the user needs to be knowledgeable enough to directly specify all of the parameters related to the release.

2.4.1.2 Environmental parameters

HPAC includes an integrated source of environmental data such as weather, terrain and land cover. The weather data from HPAC includes historical data (climatology) and single point observation (fixed wind) feature in which the wind is defined at a single point 10 m above the ground. HPAC includes a weather file editor where weather data can be manually entered and edited. It is also possible to employ external sources of weather data such as the metrological data server (MDS), which is an external data source that provides various types of weather data already formatted as HPAC files. Using the integrated weather data is quicker but generally less accurate than using external weather data.

By default, the environment used in the HPAC dispersion calculations is set to flat cultivated land, but data files which contain terrain and land cover data are integrated in the software and can be employed to increase the accuracy in the calculations. The terrain data makes it possible to use complex three dimensional surfaces representing the topographic variation at the release site. When terrain is used, HPAC will calculate a three dimensional wind field based on the weather data inputs and the specified terrain file. The wind field is determined by interpolating the weather data onto a grid and then adjusting the three dimensional field so that it satisfies mass continuity. A mass consistent wind field provides a more realistic estimate of the HPAC plume location because the model ensures that air flows around or over terrain obstacles.

The different land cover selections describes the variation of the land cover on the surface and assigns physical parameters to the transport calculation (surface roughness, canopy height, albedo, Bowen ratio) for the selected land cover type at the particular position. The differentiated land cover for the relevant project domain can be imported from the data base or directly defined in the project editor. When defining a land cover for a calculation it is important to notice that the assigned land cover will be constant throughout the release domain and not changing as the case is when the land cover data are imported from the database.

2.4.1.3 Atmospheric transport

The model used to calculate the transport of the hazardous material in HPAC is the second order closure integrated puff model (SCIPUFF), which is a Lagrangian transport and diffusion model using a Gaussian numerical puff method to represent the time dependent concentration of hazardous material by employing a three dimensional Gaussian distribution for each puff. Wind shear effects are incorporated into the model and there is defined a scheme for splitting puffs when the size exceeds a given criterion or merging overlapping puffs in the grid. This allows the model to describe multipart dispersion, such as terrain driven circulations.

Precipitation washout effects are also included for particles and droplets. SCIPUFF describes dynamic effects of buoyant rise due to thermal release of lighter-than-air materials, and also the effects of a dense cloud near the ground surface. Planetary boundary layer turbulence is represented explicitly in terms of surface heat flux and shear stress using parameterized profile shapes. The model also uses several types of meteorological input, including surface and upper air observations or three-dimensional grid data.

To ensure that the step length increases as puffs grow larger, SCIPUFF employs a time stepping scheme where the step length is determined by the turbulence time scale, advection velocity, shear distortion rates, and other physical processes. The model also use second order turbulence closure techniques to relate measurable turbulent velocity statistics to the calculated dispersion and thus get a statistical variance in the calculated concentration fields which is used in the probabilistic description of the effect display.

2.4.1.4 Output illustrating the effect of a release

After the transport calculation has been performed, HPAC can display the hazard area on a map or as a cross section of the atmosphere by showing the resulting plume or contamination as a footprint plot. The results from the calculations can also include collateral effects, like injuries and fatalities caused by exposure to the hazardous material and in this case HPAC will employ different methods for estimating the human effects for differing types of hazardous materials.

When using the footprint plots, a good estimate of where the hazardous material has been transported is the mean surface dosage plot. This plot illustrates the average realization from the defined release, but due to transport uncertainties such as atmospheric turbulence and weather, an actual event might differ from the mean prediction. This is because turbulence causes transportation of real hazard material releases to be uneven and lump whereas the mean footprint plot will be smooth. The atmospheric turbulence calculated by HPAC is used to determine the uncertainty in the direction, speed, and concentration of the plume or cloud.

To investigate the impact of changes to the source term or altered environmental data one can repeat the above stages and compare the results. For evaluating changes in the effect due to varying human protection or activity level, this can be done without repeating the transport calculation of the HPAC project.

2.4.2 ARGOS

Accident Reporting and Guiding Operational System (ARGOS) is a decision support system for enhancing crisis management for incidents involving CBRN releases from Beredskapsstyrelsen, (Danish Emergency Management Agency, DEMA), Risø National Laboratory and Prolog Development Center in Denmark. ARGOS is a prognostic tool as well as a database system for collection and presentation of data relevant for emergencies in an easily understandable form. ARGOS facilitates decision support, improved situational awareness and information sharing among the emergency response organisations. As a simulation instrument, ARGOS is also valuable for training of response organisations [13].

Originally ARGOS was developed as a decision support system for nuclear emergencies to support the Nuclear Division of the Danish Emergency Management Agency (DEMA) in dealing with emergencies related to accidents in nuclear power plants and other nuclear installations. The very first version of ARGOS was developed by Risø National Laboratory (Risø). The Danish nuclear authorities used this version during the Chernobyl accident in 1986.

The chemical part of ARGOS has been added later and includes a database with chemical substances. New models for releases from containers have been included. These cover releases of aerosols and liquids as well as evaporation of spills on the ground. A special model for dispersion of heavy gases is incorporated.

Atmospheric dispersion in ARGOS is divided in two parts, a short and mesoscale dispersion model: LSMC /RIMPUFF, and long-range models: DERMA (Danish), MLDP (Canada), SNAP (Norway) and MATCH (Sweden). For chemical releases, only the LSMC/RIMPUFF model is used [13].

The scope of the source model used in ARGOS is gas releases from industrial storages and transport containers. The source model is in fact several small models put together. Some of these models deal with the source (gaseous, liquid, or two-phase outflow; evaporation from a boiling or volatile pool) and some deal with the dispersion of dense gases from continuous or instantaneous sources (HEAVYPUFF and HEAVYPLUME). Predictions are feasible both with detailed and limited information on the release conditions. This model type is called a ‘box model’ or sometimes an ‘integral model’. The predictions are based on balances of mass and enthalpy, using thermodynamic properties of gas, air and water vapour and relatively crude parameterisation of flow and mixing processes [14]. These heavy gas models converge towards a simple distribution without density effects. After 1 km, ARGOS automatically changes to use RIMPUFF which handles this phase more exact [15]. The communication with the main ARGOS system is based on XML and text files.

New features underway in ARGOS cover explosions such as Radiological Dispersal Devices (RDD or so-called dirty bombs) and primitive nuclear weapons or improvised nuclear devices (IND). It also covers handling of several simultaneous releases; this could be necessary for terror situations. To facilitate dispersion calculations in urban areas, a new urban dispersion puff model

(Urban Release and Dispersion, URD) is under development within the ARGOS framework. This work is lead by the Technical University of Denmark (Risø) and Totalförsvarets forskningsinstitut (FOI) in Sweden is developing a wind flow model for use in URD.

ARGOS integrates currently with a number of external models:

- The atmospheric dispersion model “Risø Meso-scale Puff Model” (RIMPUFF) for calculating local-scale dispersion forecasts,
- various long-range atmospheric dispersion models running remotely on meteorological computing centres,
- the “Food and Dose Module” (FDM) model for calculating doses in rural areas,
- the “European Radiological Model for Inhabited Areas” (ERMIN) for calculating doses in an urban environment and,
- the STRATEGY food-chain countermeasure model developed under the European Commissions Fifth Framework programme
- a Risø developed model for calculating chemical release source terms from containers based on a specification of the release geometry and temperature,
- a Risø developed model for calculation of dispersion of heavy gases,
- the “Urban Release and Dispersion (URD)” model (see above)

ARGOS is an open platform with models attached as loose-coupled modules to the system. This construction makes it easy to adopt new models for enhancement of the system, and helps to keep ARGOS up-to-date and flexible for using models that has a preference in individual countries. A disadvantage of such an arrangement is that many contributors from different organisations might slow down the development process and make the software somewhat difficult to use.

Version 8.3 of ARGOS has been used for the simulations in this report. A new version (version 9.0) is now available. According to DEMA, one of the improvements in the RIMPUFF module give gas plumes with smaller widths and longer maximum travel distances [16].

2.4.3 DEGADIS

DEnse GAs DISpersion (DEGADIS) is a mathematical dispersion model for toxic chemical gases and/or aerosols developed for the U.S. Environmental Protection Agency [17]. It is a box model which describes a gas plume collapsing under gravity. Its range of applicability includes continuous, instantaneous, finite duration, and time-variant releases; negatively-buoyant and neutrally-buoyant releases; ground-level, low-momentum area releases; and ground-level or elevated upwardly-directed stack releases. DEGADIS was originally designed to model dense gas (or aerosol) clouds released with zero initial momentum. However, a jet-plume model has been interfaced with DEGADIS to provide vertically oriented gas or aerosol jets.

DEGADIS can model the dispersion from a steady-state source release or a transient release. Steady-state releases are modelled as a series of transient source calculations carried out until the source characteristics does not change significantly with time. Transient releases are carried out as a series of pseudo-steady-state releases.

DEGADIS describes the dispersion processes which accompany the gravity-driven flow and entrainment of gas into the atmospheric boundary layer, and the dispersion downwind. The vertical dispersion is modelled by a power-law, while the horizontal dispersion is modelled by a modified Gaussian profile with a power-law specification for the wind profile.

The model simulates only one set of meteorological conditions, and therefore should not be considered applicable over time periods much longer than 1 or 2 hours. The simulations are carried out over flat, unobstructed terrain for which the characteristic surface roughness is not a significant fraction of the depth of the dispersion layer. The model does not characterize the density of aerosol-type releases; rather, the user must assess that independently prior to the simulation.

DEGADIS does not have a graphical user interface like HPAC and ARGOS. Instead it is text based and the simulation is performed by running batch files.

DEGADIS consists of several programs. First, there is a program for creating an input file and an executable batch file. There are different programs for setting up ground level release and elevated jet release. These programs prompt the user for input values to the different variables for the particular simulation. This includes description of the source (release rate from a container, evaporation rate from a pool, etc). The user will also need to specify a lower and an upper level of concern for the concentration. These variables are written to an input file. This input file can be written “by hand”; if the user wishes to change some parameters it can be more efficient to change them directly in the input file, instead of executing the DEGADIS input program again.

The executable batch file then calls the relevant DEGADIS programs. These include programs for calculating the widths of the clouds containing concentration levels corresponding to the lower and upper level of concern at various distances downwind or points in time after the release. The dispersion of the cloud is modelled until the concentration is half of the lower level of concern. Also this batch file can be written from scratch by the user.

The output from DEGADIS is a text file. In order to produce graphics plots another computer program, like Excel or MATLAB, must be used.

2.5 Meteorology and surface roughness

2.5.1 Meteorology

There are many meteorological parameters which affect the evaporation and dispersion of chemicals from a release. Some important meteorological parameters are temperature, relative humidity, wind speed and direction. Another important parameter is the atmospheric stability. This parameter defines the vertical mixing of the air and depends both on the temperature profile from the ground and upward, and the vertical variation of the wind field (which again depends on among other parameters, time of day, time of year, cloud cover, etc). The air stability categories are: A very unstable, B unstable, C slightly unstable, D neutral, E stable, and F very stable.

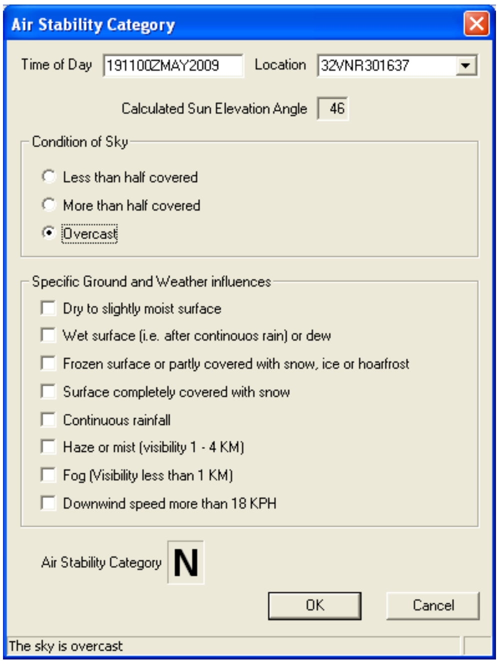
In meteorology, an okta is a unit of measurement used to describe cloud cover. Sky conditions are estimated in terms of how many eighths of the sky are obscured by cloud, ranging from completely clear, 0 oktas, through to completely overcast, 8 oktas. In addition, the cloud cover indicator '9' indicates that the sky is obscured, usually due to dense fog or heavy snow [18].

The relation between atmospheric stability and time of day, wind speed and cloud cover is given in Table 2.2.

	DAY Incoming solar radiation			NIGHT	
Wind speed (m/s)	Strong	Moderate	Slight	> 4/8 cloud	< 3/8 cloud
< 2	A	A - B	B		
2 - 3	A - B	B	C	E	F
3 - 5	B	B - C	C	D	E
5 - 6	C	C - D	D	D	D
> 6	C	D	D	D	D

Table 2.2 Air stability classes. Based on D. Bruce Turners Workbook of Atmospheric Dispersion Estimates [19].

NBC-Analysis has its own software tool to estimate the atmospheric stability based on time of day, geographical location, cloud cover and some other specific influences (see Figure 2.1). The output is the air stability category: Unstable, Neutral or Stable.



Air Stability Category

Time of Day 191100ZMAY2009 Location 32VNR301637

Calculated Sun Elevation Angle 46

Condition of Sky

○ Less than half covered
○ More than half covered
● Overcast

Specific Ground and Weather influences

☐ Dry to slightly moist surface
☐ Wet surface (i.e. after continouos rain) or dew
☐ Frozen surface or partly covered with snow, ice or hoarfrost
☐ Surface completely covered with snow
☐ Continuous rainfall
☐ Haze or mist (visibility 1 - 4 KM)
☐ Fog (Visibility less than 1 KM)
☐ Downwind speed more than 18 KPH

Air Stability Category N

The sky is overcast

Figure 2.1 Tool to estimate air stability used by NBC-Analysis [20].

The meteorological conditions will vary with height above ground and with the distance from the release point. It is therefore important to have meteorological data for several positions throughout the computational domain in order to predict the hazard area as correctly as possible. The different hazard prediction programs have different ways to represent the meteorological conditions and require different input parameters. The meteorological parameters needed are not easy to access by the user without assistance from meteorological services. In order to use the software efficiently it will therefore be necessary to import weather forecasts and weather reports from meteorological stations in the area of concern. This should preferably be done automatically in order to have the data rapidly when needed by the user. It is not practically useful to import weather date manually in an operational use of the programs. This could, however, be done by expert users for planning purposes.

2.5.2 Surface Roughness

The dispersion depends very much on the geometrical properties of the surface over which the cloud travel. A rough surface increases the frictional forces and thus also the vertical mixing of the momentum and concentration fields. A surface roughness parameter is therefore defined to represent different surfaces. This parameter is most often included in the data from the map used by the different hazard prediction models. A table with different surface roughness values is shown below (Table 2.3).

Land cover	Spring	Summer	Fall	Winter
Urban	1.00	1.00	1.00	1.00
Agricultural	0.03	0.20	0.05	0.01
Rangeland	0.05	0.10	0.01	0.001
Deciduous forest	1.00	1.30	0.80	0.50
Coniferous forest, wetland	1.30	1.30	1.30	1.30
Mixed forest	1.15	1.30	1.05	0.90
Water	0.0001	0.0001	0.0001	0.0001
Barren land	0.002	0.002	0.002	0.002
Non-forested wetlands	0.20	0.20	0.20	0.05
Mixed agricultural/range	0.04	0.15	0.03	0.006
Rocky (with low shrubs)	0.30	0.30	0.30	0.15

Table 2.3 Surface Roughness (in meters) by land cover and season [21]. In this table, winter is defined for conditions where there is snow present; winter months with no snow are assigned to the fall category.

This table lists some typical values for the surface roughness parameters on various land covers. In the calculations however, these are not necessarily the values used as other values have also been published. For instance SCIPUFF (the puff model used by HPAC) uses other values for the surface roughness.

In addition to the surface roughness taken from the map data, ARGOS needs the surface roughness around each meteorological tower to be able to define the wind profile.

3 Source modelling

Source modelling is a description of the release of the hazardous compound into the atmosphere. This includes the characteristics of the release of fluid from a tank: the phase of the fluid (the ratio of liquid to vapour in the jet), and other physical and chemical characteristics of the out flowing jet. Also evaporation from a pool is included in the source modelling term.

This chapter gives a brief overview of the source modelling performed for the scenarios including the toxic industrial chemicals chlorine and ammonia.

3.1 Flashing

The amount of liquid that flashes depends on the temperature. The TNO Yellow Book [22] gives the following equation for estimating this amount:

$$\theta_f = \theta_0 \frac{T_b}{T_0} + \frac{T_b}{L} C_{p,l} \ln \frac{T_0}{T_b}$$

where θ_f is the mass fraction that flashes, θ_0 the mass fraction of vapour in the storage tank, T_b and T_0 the boiling and storage temperature (in Kelvin), L the latent heat at the boiling temperature, and $C_{p,l}$ the specific heat of the liquid. For these calculations, it is assumed that the initial mass fraction of vapour is zero. This is not true; the pressurized tanks are never completely filled with liquid (for security reasons). However, this factor is very small compared to the second factor in the equation. It is assumed that the mass fraction of airborne aerosols is equal to the mass fraction of gas from flashing [22], the rest of the released liquid forms an evaporating pool on the ground.

If a tanker truck contains a total of 20 tons pressurized chlorine at ambient temperature (15 °C), based on the formula above, when the tanker explodes, 3 000 kg (15 %) evaporates immediately. An initial airborne plume containing 3 000 kg vapour and 3 000 kg aerosol droplets is then formed. The remaining 14 000 kg liquid chlorine forms a pool at the boiling temperature on the ground, which will evaporate and form a secondary cloud. This vaporization process is slower than the initial, immediate evaporation process. The pool is assumed to have a depth of one centimetre (which corresponds to normal sandy soil, gravel, railroad yard, [22]) and thereby a surface area of 900 square meters (circular with radius 17 meter).

3.2 Pool evaporation calculations

3.2.1 Yellow Book (as input to DEGADIS)

The time varying evaporation rate from the pool, $q(t)$, is calculated by:

$$q(t) = \frac{H_c(t)+H_a}{L_v(T_b)} A\,,$$

where $H_c(t)$ and H_a are the heat fluxes from the subsoil and the air, $L_v(T_b)$ is the latent heat of vaporisation at the boiling temperature T_b, and A is the area of the pool. The latent heat is a temperature dependent parameter of the evaporating substance, while the heat flux is a property of the subsoil and the surrounding air. The heat flux from the subsoil is calculated by:

$$H_c(t) = C_R \lambda_s (T_{s,0} - T_b) / \sqrt{a_s \pi t} \, ,$$

where C_R is a correction term to reflect freezing of the water in the subsoil, λ_s is the thermal conductivity of the subsoil, a_s the thermal diffusivity of the subsoil, and $T_{s,0}$ the initial subsoil temperature. The thermal diffusivity is related to the thermal conduction and the specific heat of the subsoil, C_s, by:

$$a_s = \frac{\lambda_s}{\rho_s C_s} \, ,$$

where ρ_s is the density of the subsoil.

The heat flux from the air above the pool is given by[4]:

$$H_a = k_{H,a}(T_a - T_b) \, ,$$

where T_a is the ambient temperature and $k_{H,a}$ the heat transfer coefficient to the atmosphere. The heat transfer coefficient can be estimated by:

$$k_{H,a} = \frac{\lambda_a Nu}{2r} \, ,$$

where λ_a is the thermal conductivity of air, $2r$ a characteristic length of the pool (in these calculations it is set equal to the pool diameter), and Nu the Nusselt number, which can be expressed by the Reynold’s number (Re) and Schmidt’s number (Sc) by:

$$Nu = 0.037 Sc^{1/3} \mathrm{Re}^{0.8}$$
$$\mathrm{Re} = U(2r) / \nu$$
$$Sc = \nu / D_a$$

U is the air velocity, ν the kinematic viscosity of air, and D_a the thermal diffusivity. For air, the Schmidt number is: $Sc \approx 0.8$.

Figure 3.1 shows the calculated evaporation rate from the chlorine pool described above, when the ambient conditions are as described in Chapter 4.5. The temperature of the soil is taken to be that of air (14.2 °C). The evaporation rates calculated with heat flux from only the ground and atmosphere are also shown. Initially the heat flux from the subsoil is dominating, but after some time, heat flux from the air becomes comparable and even dominating.

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[4] The TNO Yellow Book [22] also lists other formulas for calculating the heat flux from the air, which give quite different results. A comparison between different methods, and an assessment of which method would give the most accurate result, are not given in this report. This formula is given as an example.

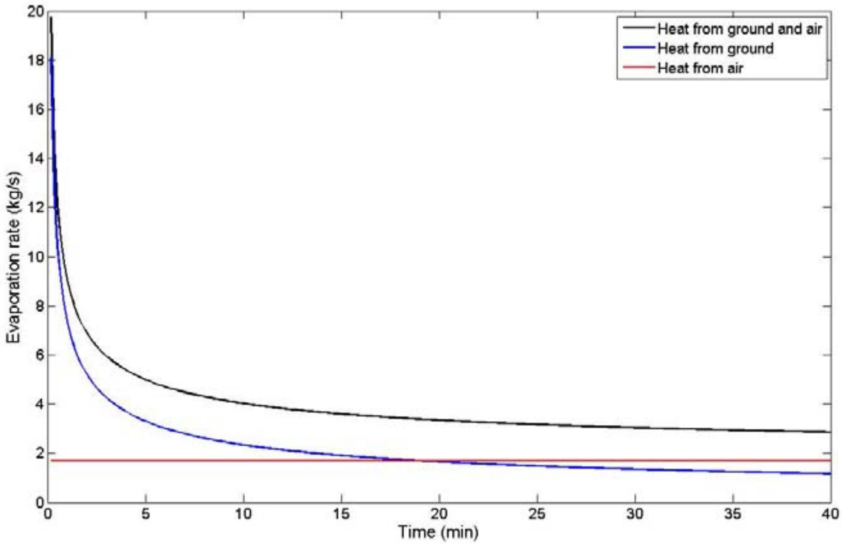

Figure 3.1 The evaporation rate from a chlorine pool with area 900 m^2 as function of time. The calculated evaporation rate with only heat flux from the surrounding air, H_a *(red), only from the ground,* H_c *(blue), and the total rate (black) are shown.*

The heat flux from the air gives a constant evaporation rate. This will not be completely correct. Firstly, it is assumed that the temperature of the air above the pool does not decrease. This is a simplification as the temperature of the air will decrease because heat is taken from the air by the evaporation process. Secondly, the evaporation rate will decrease toward the end as the area of the pool decreases. (The figure shows the evaporation rate for the first 40 minutes only.)

Figure 3.2 shows the evaporated mass from the pool as function of time as calculated with the evaporation rates shown in Figure 3.1 with combined heat from the ground and air and heat only from the ground. It is clearly seen that the evaporation rates are equal in the first minutes. However, after some time heat from the air stream is dominant. With only heat from the ground, the pool will evaporate in about four hours, but when heat from the passing air is included, the evaporation time decrease to about one hour[5].

As mentioned above, however, the evaporation rate will decrease toward the end. Thus the time for the evaporation would be somewhat larger than shown in the figure, and in reality the curves for the evaporated mass will flatten out when approaching 14000 kg (the original mass of the pool).

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[5] As mentioned in footnote 4, there are other methods for calculating the heat flux from air, which would alter the results somewhat.

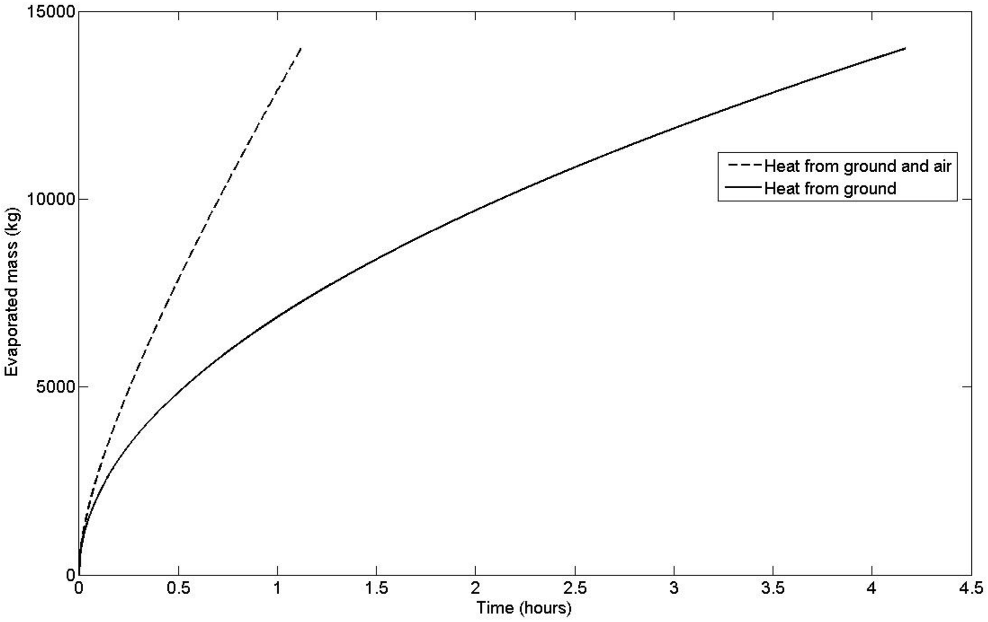

Figure 3.2 Evaporated mass from a chlorine pool as a function of time, for combined heat transfer from the air and the ground, and from the ground only.

3.2.2 ARGOS

The pool evaporation in ARGOS assumes heat transfer mainly from the surface beneath the pool, but also from the air and from short-wave and long-wave radiation. The portion of the total heat flux of the radiation depends on solar angle, cloud coverage and other external conditions. However, for cryogenics, thermal conduction from the surface beneath the pool will be dominating [23].

ARGOS computes the heat flux from the pool basin as heat diffusion from a semi-infinite solid with uniform material properties and no porosity. The thermal conduction from the surface, λ_s, is described by the ordinary heat conduction equation [23]:

$$\rho_s C_s \frac{\partial T}{\partial t} = \lambda_s \frac{\partial^2 T}{\partial z^2},$$

where ρ_s is the density of the soil, C_s is the heat capacity of the soil, and z is the depth into the subsoil. From this, an expression for the heat flux is found:

$$H_c(t) = \lambda_s \frac{\partial T}{\partial z},$$

which, for constant surface temperature, is simplified to:

$$H_c(t) = \Delta T \sqrt{\frac{\lambda_s \rho_s C_s}{\pi t}}.$$

This is the same formula for the heat flux as in the TNO Yellow Book, except that the Yellow Book equation includes a factor to account for freezing of water in the subsoil.

The evaporation mass flux is then calculated by dividing the heat, $H(t)$, by the latent heat of evaporation.

3.2.3 HPAC

The mass transfer rate, q, in the HPAC calculation of pool evaporation is given by the Sherwood number:

$$Sh = \frac{q}{DWC_0},$$

where D is the diffusivity of vapour in air, W is a width of an equivalent square pool ($W=\pi^{1/2}R$, where R is the radius of the circular pool), and C_0 the saturation concentration. HPAC uses expressions for the Sherwood number from the HGSYSTEM [24] for calculating the evaporation rate:

$$Sh = 0.664 Sc^{1/3}\,\mathrm{Re}_W^{1/2} \qquad ;\mathrm{Re}_W < 3.2\cdot 10^5$$
$$Sh = 0.037 Sc^{1/3}(\mathrm{Re}_W^{4/5} - 15200)\ ;\mathrm{Re}_W \geq 3.2\cdot 10^5,$$

where the Reynold's number based on the wind speed, U, is:

$$\mathrm{Re}_W = \rho_a U W / \mu_a,$$

and the Schmidt number:

$$Sc = \frac{v_a}{D},$$

where ρ_a, v_a and μ_a are the density and the kinematic and dynamic viscosity of air respectively.

This mass flux (evaporation rate) is coupled to the heat fluxes by the latent heat of evaporation:

$$q = \frac{H_s + H_a}{L(T_b)}.$$

The heat to the evaporation process are taken from heat conduction to the ground and convected heat flux from the air by similar expressions as for the Yellow Book calculations:

$$H_s = \frac{\lambda_s W^2 (T_{s,0} - T_p)}{\sqrt{a_s \pi t}}$$
$$H_a = Nu \lambda_a W (T_a - T_p),$$

where T_p is the pool temperature (not necessarily equal to the boiling temperature) and the ambient temperature, T_a, is taken 10 meters from the pool. These are also equal to the Yellow Book formulas, except the correction factor for freezing of water in the subsoil. From the last three equations, the pool temperature is calculated.

The physical properties of the underlying surface are taken to be that of sand.

3.3 Comparison of methods for evaporation rate calculations

The three methods, Yellow Book, ARGOS and HPAC, are quite similar. HPAC starts with calculating the mass transfer to the surrounding air based on a dimensionless measure of mass transfer rate and then updates the temperature of the pool from the heat fluxes, while Yellow Book and ARGOS calculates the rate from the heat transfer from the subsoil. Also HPAC and Yellow Book take heat both from the surrounding air and the subsoil, while ARGOS (for cryogenics) ignores heat from the ambient air. In ARGOS it is possible to specify the substance of the subsoil, with Yellow Book the user can use any material he/she desires, while HPAC takes the physical properties of the soil to be that of sand.

The evaporation rates from a chlorine pool on a surface of sandy soil is calculated by using the programs ARGOS, HPAC and the formulas given in Yellow book. A comparison of the rates is shown in Figure 3.3.

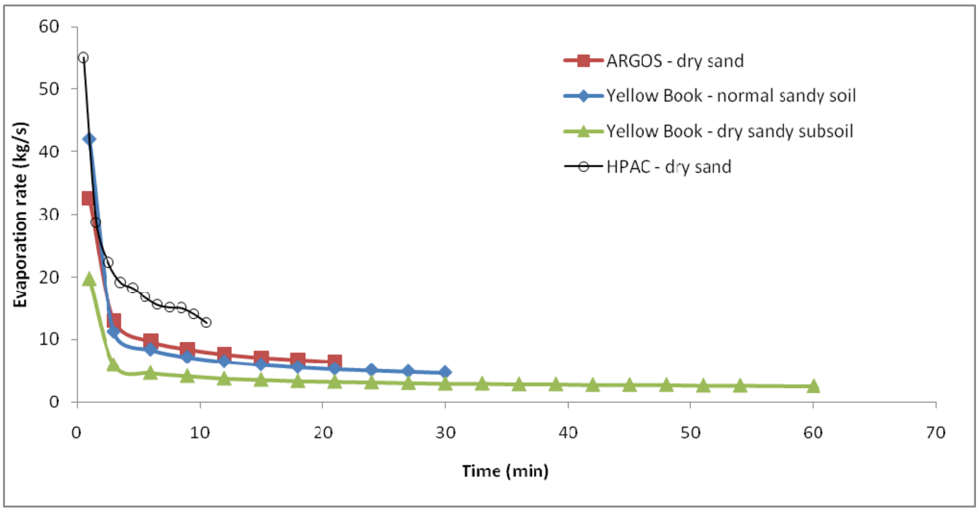

Figure 3.3 Comparison of evaporation rates of chlorine from different surfaces calculated from Yellow Book and ARGOS source term module, in addition to data from HPAC.

From Figure 3.3, we see that HPAC predicts the highest evaporation rate and Yellow Book has predicted the lowest evaporation rate (about half the rate predicted by HPAC). The rate predicted by ARGOS is in the middle of this range. The equations solved in the three approaches are similar, and the cause of the large differences is probably that different parameters for the thermal properties of the subsoil are used.

In the figure, the evaporation rates do not approach zero, but flattens out at some level until the evaporation process is abruptly cut off when all the liquid is evaporated. This is obviously not correct; the evaporation rates must approach zero. This discrepancy is partly explained by the fact that the area of the pool is considered to be constant throughout the evaporation process in these calculations. In reality, however, the area will decrease, and the original large pool will furthermore at some point be divided into areas with liquid and bare land, and this will lead to a decrease in the evaporation rate.

4 Modelling and simulation results for chlorine release

4.1 Scenario description

The initial comparison of the different models and programs was carried out with Ørland Main Air Station (MAS) as a test location. Ørland was chosen because a meteorological tower with downloadable data from this location is present[6], and also because of the relatively diverse weather conditions and surrounding land covers (both land and sea, see Table 4.1).

1a	Ørland	Chlorine	Different terrain (land and sea)
1b	Ørland	Chlorine	Meteorological data from two heights
1c	Ørland	Chlorine	Source term modelling included

Table 4.1 Chlorine release scenarios.

We assume that chlorine is released as a result of total rupture of a pressurised tank. During such a release of pressure-liquefied gas, a fraction of the liquid evaporates immediately (flashing), some liquid is dispersed as aerosols (airborne droplets), while the rest of the liquid forms an evaporating pool on the ground [22]. Explanation of the calculations performed to obtain the amount of mass that is airborne and also the evaporation rate from the pool, are given in Chapter 3.

This scenario constitutes a chlorine release from a tanker truck containing 20 000 kg liquefied chlorine during day-time (at 1100Z). According to calculations using the TNO Yellow Book 6 000 kg is released as gas and aerosol droplets and 14 000 kg forms a pool of liquid on the ground (see Table 4.2). Meteorological input parameters are shown in Table 4.3 (in Chapter 4.4.1). The toxicity threshold concentration limits used for chlorine (estimated for an exposure time of 10 min) are the Acute Exposure Guideline Levels (AEGL) and the Immediately Dangerous to Life and Health (IDLH): AEGL-1[7] = 1.5 mg/m^3, AEGL-2[8] = 8.1 mg/m^3, IDLH[9] = 29.5 mg/m^3, AEGL-3[10] = 145 mg/m^3 [25;26].

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[6] www.esrl.noaa.gov/raobs/, accessed at 26 February 2010

[7] AEGL-1 is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

[8] AEGL-2 is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

[9] IDLH = The threshold concentration “immediately dangerous to life and health” (IDLH) identified by the National Institute for Occupational Safety and Health (NIOSH).

[10] AEGL-3 is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Parameter	Value
Time of day	1100Z
Position (MGRS)	32VNR 30156376
Compound released	Chlorine
Amount released (total)	20 000 kg
Released as gas and aerosol	6 000 kg
Released as liquid	14 000 kg
Toxicological limits	
AEGL-1	1.5 mg/m^3 [25]
AEGL-2	8.1 mg/m^3 [25]
IDLH	29.5 mg/m^3 [26]
AEGL-3	145 mg/m^3 [25]

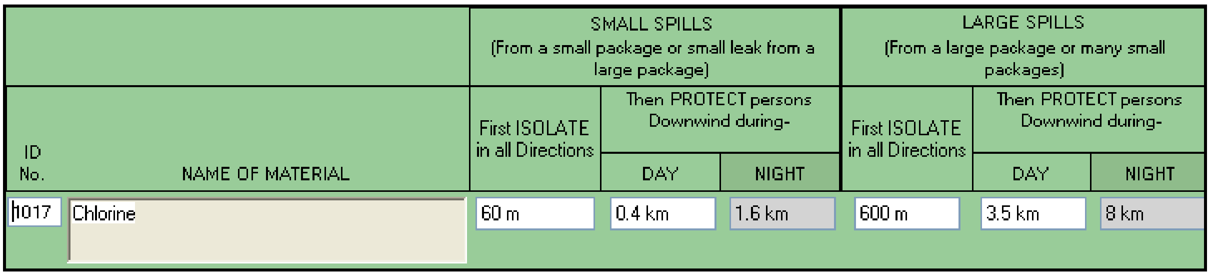
Table 4.2 Input parameters.

4.2 Hazard prediction and assessment tools

First, the hazard areas predicted by the Emergency Response Guidebook (ERG2008) from CANUTEC, and the “Farlig gods” program from DSB were obtained. The results are presented in this section.

4.2.1 Emergency Response Guidebook

The Emergency Response Guidebook (ERG 2008) was used to estimate the size of the initial isolation zones and the protective action distances (PAD, the distance in which protective actions should be considered) for the release of chlorine. The printout of chlorine release from ERG2008 is shown in Figure 4.1 below.



ID No.	NAME OF MATERIAL	SMALL SPILLS (From a small package or small leak from a large package)			LARGE SPILLS (From a large package or many small packages)		
		First ISOLATE in all Directions	Then PROTECT persons Downwind during-		First ISOLATE in all Directions	Then PROTECT persons Downwind during-	
			DAY	NIGHT		DAY	NIGHT
1017	Chlorine	60 m	0.4 km	1.6 km	600 m	3.5 km	8 km

Figure 4.1 Printout of chlorine release from ERG2008.

The distances in ERG2008 are given for small spills (less than 200 litres for liquids and 300 kg for solids) and for large spills (greater than 200 litres for liquids and 300 kg for solids), separately. Different isolation zones and PADs are given for day-time and night-time releases. The chlorine release discussed in the current report is defined as a large spill occurring during day-time. According to ERG2008, one should first isolate **600 m** in all directions around a large spill of chlorine and then protect persons **3.5 km** downwind during daytime.

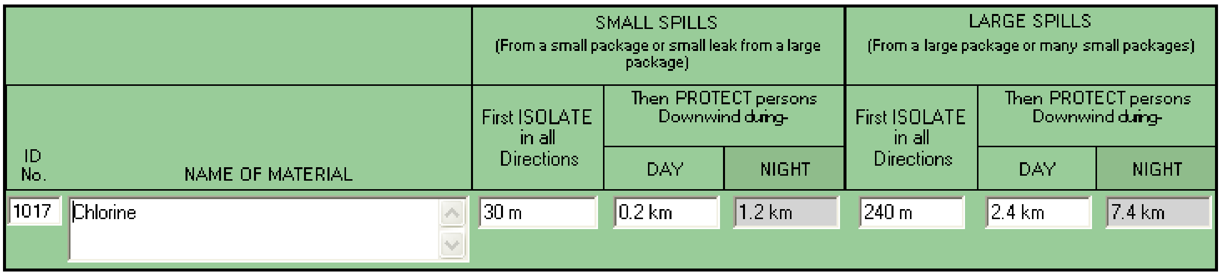
4.2.2 DSB ”Farlig gods”

The “Farlig gods” program from DSB gives a safety distance of **484 m** for chlorine at a temperature of 10 °C. It should be noted that DSB recommends that this function is applied with caution, and that the method should be limited to toxic gases and large accidents (tanker trucks and rail wagons). The safety distances are guidelines only and intended for the acute phase. The method is simple, and temperature is the only required input parameter. The program calculates the vapour pressure at this given temperatures, and it is assumed that the vapour pressure in kPa corresponds directly to a recommended safety distance (1 kPa = 1m).

4.3 NBC-Analysis

In NBC-Analysis, the user can choose between a release from a tanker truck or from an industrial storage site. The amount released is assessed as very different in the two situations and the hazard area is much larger in the case of release from an industrial site. In the current scenario, a release from a tanker is assumed.[11]

In case of a Toxic Industrial Material (TIM) released from a transport vehicle, the data given by NBC-Analysis are taken from the 2004 version of ERGO. One should note that the size of the initial isolation zones and the protective action distances for chlorine are different in the 2004 version of ERGO used by NBC-Analysis compared to the current 2008 version of ERGO. The distances given by NBC-Analysis are shown in Figure 4.2.



		SMALL SPILLS (From a small package or small leak from a large package)			LARGE SPILLS (From a large package or many small packages)		
ID No.	NAME OF MATERIAL	First ISOLATE in all Directions	Then PROTECT persons Downwind during- DAY	Then PROTECT persons Downwind during- NIGHT	First ISOLATE in all Directions	Then PROTECT persons Downwind during- DAY	Then PROTECT persons Downwind during- NIGHT
1017	Chlorine	30 m	0.2 km	1.2 km	240 m	2.4 km	7.4 km

Figure 4.2 Printout of chlorine release from ERG2004 used by NBC-Analysis.

NBC-Analysis produces a circular “release area”, which is the predicted area immediately affected by the release (equals the initial isolation zone from ERGO). In the current scenario (a large day-time release), a circular release area with radius **240 m** is predicted. Secondly, NBC-Analysis produces a “hazard area”, in which unprotected personnel may be affected by the agent spreading downwind from the “release area”. In case of an extra large spill (defined as greater than 1500 kg), the protective action distance given in ERGO should, according to NBC-Analysis, be doubled. The hazard area from NBC-Analysis in the current scenario has a triangular shape which extends **4.8 km** downwind (see Figure 4.3). The area affected is 30 degrees on each side of the centreline.

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[11] If a release from a production plant is assumed instead of from a transport vehicle, the affected area estimated by NBC-Analysis is no longer based on ERGO. The area in this case is much larger, i.e. up to 30 km downwind at the current weather situation.

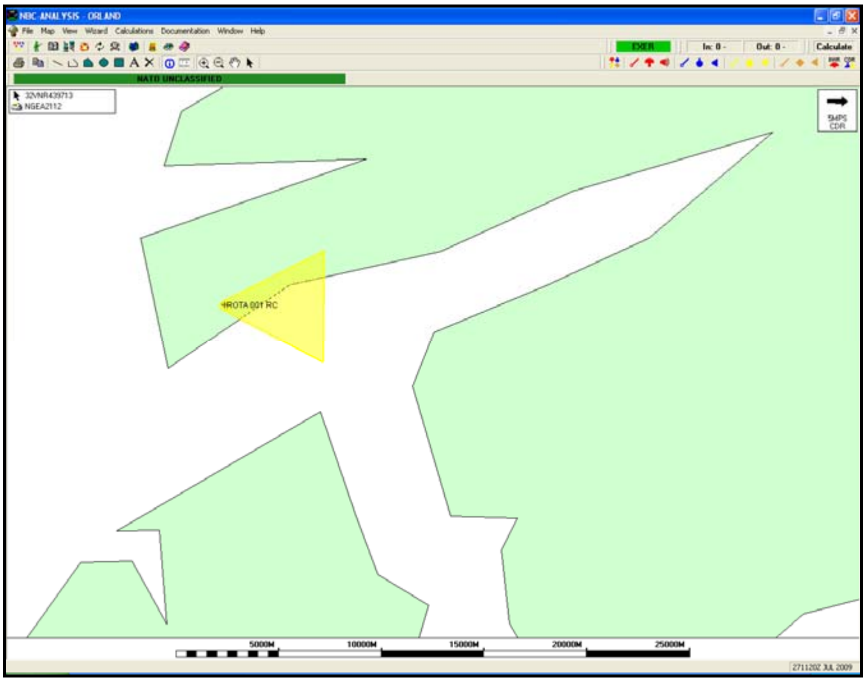

Figure 4.3 Plot of the chlorine hazard area made by NBC-Analysis from a release at Ørland MAS during day-time.

4.4 Simple meteorological conditions

4.4.1 Dispersion modelling and simulation

It was decided to start the comparison of HPAC, ARGOS and DEGADIS with very simple release and weather input data and then increase the complexity. The comparison therefore started with a release consisting only of chlorine in vapour state, starting after it has been dispersed into gaseous state from a total rupture of a tank. That is, first we consider only the initial plume and treat this as consisting only of gas.

The three softwares we have tested differ with respect to minimum release times. In HPAC an instantaneous release can be defined, while in ARGOS it is not possible to define releases that last less than one minute. It is possible to model an instantaneous release by DEGADIS, but a release time of one minute for the initial cloud was used to be able to compare the results with the results from HPAC and ARGOS.

The input parameters from this first comparison are given in Table 4.3. In HPAC, the release was defined using the analytic module. In this module, one could either define only wind speed and direction in one point (called “Fixed wind”) or define all available weather parameters manually (called “manual weather”). In the manual weather module, one can define several weather stations within the computational domain. This has not been done in our simulations where only the weather data from the meteorological tower measurements have been used.

Input parameter	Value	HPAC-1 (fixed wind)	HPAC-2 (manual weather)	ARGOS	DEGADIS
Released gas	Chlorine	X$^{3)}$	X	X	X
Released amount	6000 kg - vapour	X	X	X	X
Release rate	60 sec 100 kg/s	X	X	X	X
Surface roughness	0.1 m (grassland) 0.0005 m (water) [12]	X	X	From map$^{2)}$	X
Wind speed (at 5 m height)	3 m/s	At 10 m	X	X	X
Temperature (at 0 m height)	10 °C	Automatic	X	X	Surface
Temperature (at 5 m height)	10 °C	Automatic	X	At 2 m height	Air
Cloud cover (octavos)$^{1)}$	Overcast (8)	X	X	X	NA$^{4)}$
Atmospheric stability category		Not used	Not used	NA	D (Neutral)
Precipitation (mm)	0 mm	X	X	X	NA
Relative humidity (RH)	80 %	Automatic	X	X	X
Pressure	101325 Pa	Automatic	X	X	X
Release height	2 m	X	X	Ground level	Ground level
Sampling height (z)		Surface	Surface	Surface	1.6 m

Table 4.3 Input parameters for the first comparison with chlorine.
$^{1)}$ Cloud cover is measured in octavos (1-8, and 0=clear sky)
$^{2)}$ Surface roughness at the meteorological tower is set to 0.1 m
$^{3)}$ X: Used by the program
$^{4)}$ NA: Not applicable

In HPAC the concentration footprint plots were used to determine the maximum length, width and height with one minute intervals. Horizontal slices at ground level were used to estimate the maximum length and width, while vertical slices downwind were used to estimate the maximum height of the plume for the respective toxicity levels.

In ARGOS, a graphical plot is given as a result of each run. One can select different types of plots; the instantaneous concentration plot and the maximum instantaneous plot[12] are the most useful for TIC releases where the toxicity is little dependent of the exposure time. The maximum distance travelled and the maximum width of the plume has been measured manually by using the distance tool in the software.

The output of DEGADIS is a text file which includes (among more) the concentration at the centreline downwind of the release. If a transient release is modelled, the file also lists the width of the plume for specified concentration levels at certain time steps. The concentration levels, the

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[12] Instantaneous concentration plot gives the concentration in each point for each time step (in mg/m^3 or ppm). Maximum instantaneous plot gives the maximum concentration (in mg/m^3 or ppm) in each point independent of the time when this concentration appears.

sampling height in which the concentration levels are given, and the time steps (both the first time step, the range between the time steps and the number of time steps) can be specified by the user. The height of the cloud is not given automatically by DEGADIS.

Vignette 1: Wind from 270 degrees

In the first vignette, the wind direction was chosen from west towards east (from 270 degrees). The results from HPAC are shown in Figure 4.4 - Figure 4.7 and from ARGOS in Figure 4.8 - Figure 4.9. The DEGADIS program does not take the surface into consideration, except for the roughness parameter, and this parameter is constant over the computational domain. DEGADIS has therefore not been used with wind from west, because the terrain towards east is a combination of sea and land.

Figure 4.4 is taken from the simulation with HPAC-1 parameters. Plots from HPAC-2 are not shown because it gives very similar results compared to HPAC-1. The figure shows the horizontal concentration profiles at the time steps when the concentration drops below the concentration levels used in the report (AEGL-3, IDLH, AEGL-2 and AEGL-1).

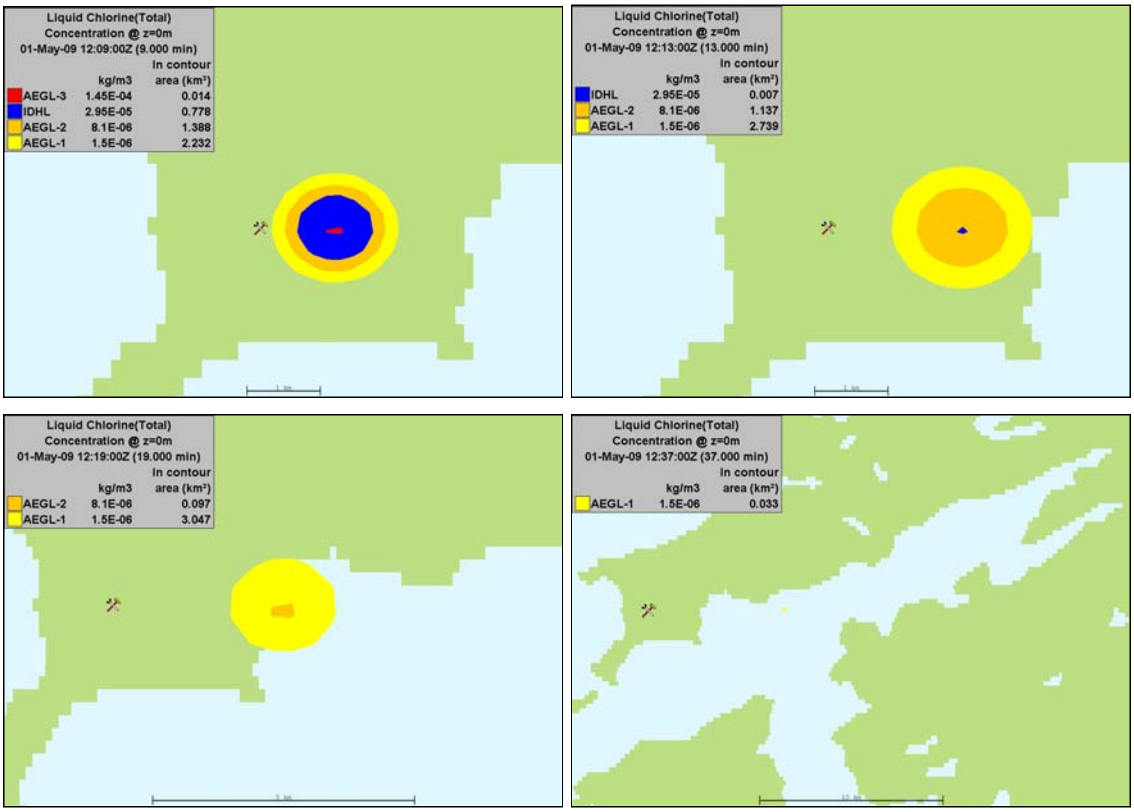

Figure 4.4 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC (fixed wind module). The wind speed is 3 m/s from west. The situation shown is the time when the concentration drops below AEGL-3 level (9 min)(upper left), IDLH level (13 min) (upper right), AEGL-2 level (19 min) (lower left) and AEGL-1 level (37 min) (lower right).

Figure 4.5 shows the total area affected by the specified threshold concentration levels. Note that this figure does not show the concentration variations with time; hence, the whole area will not be affected simultaneously. The next figure (Figure 4.6) shows the vertical concentration profiles obtained by HPAC. Again, only the results using the fixed wind module (HPAC-1) are shown.

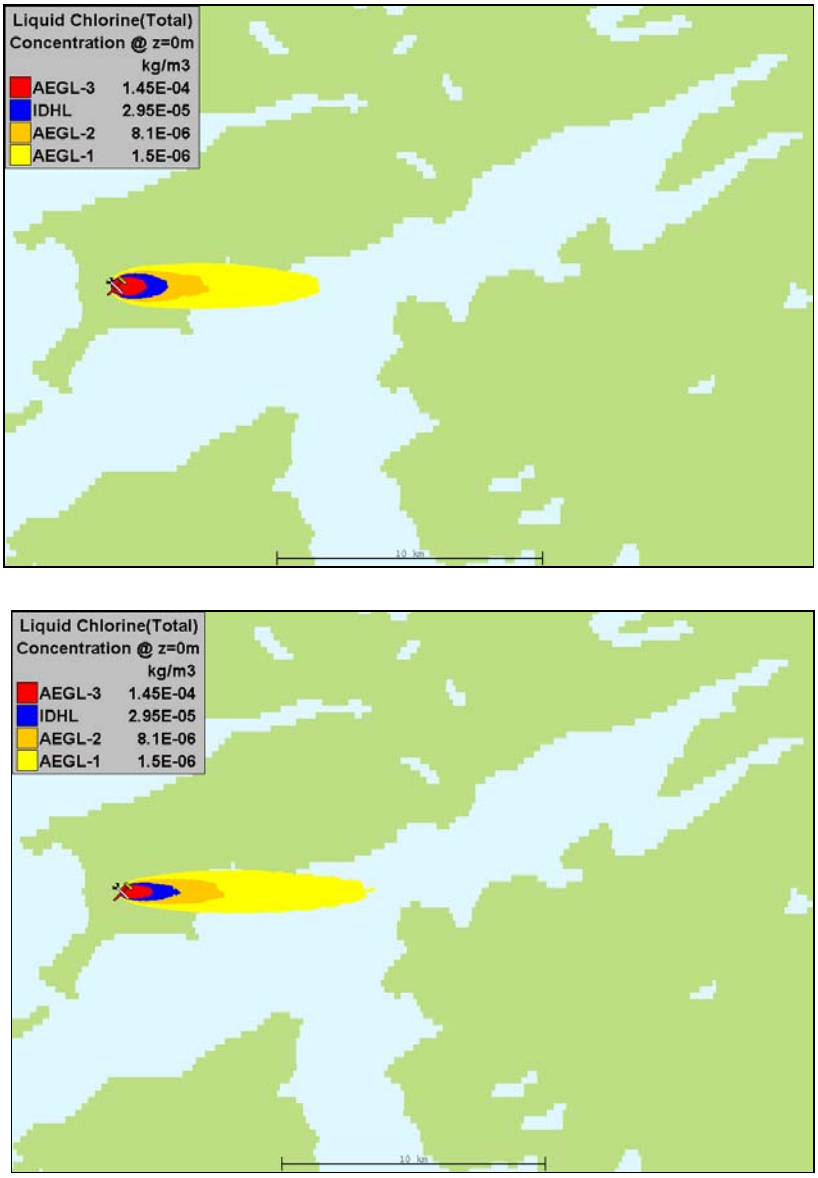

Figure 4.5 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC. The wind speed is 3 m/s from west. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3) for both the fixed wind weather module (HPAC-1)(top) and the manual weather module (HPAC-2)(bottom).

In the next figure (Figure 4.7), the total area in the vertical plane affected by the specified concentration level is shown. Note that the figure does not show the concentration variation with time and that the whole area will not be affected simultaneously.

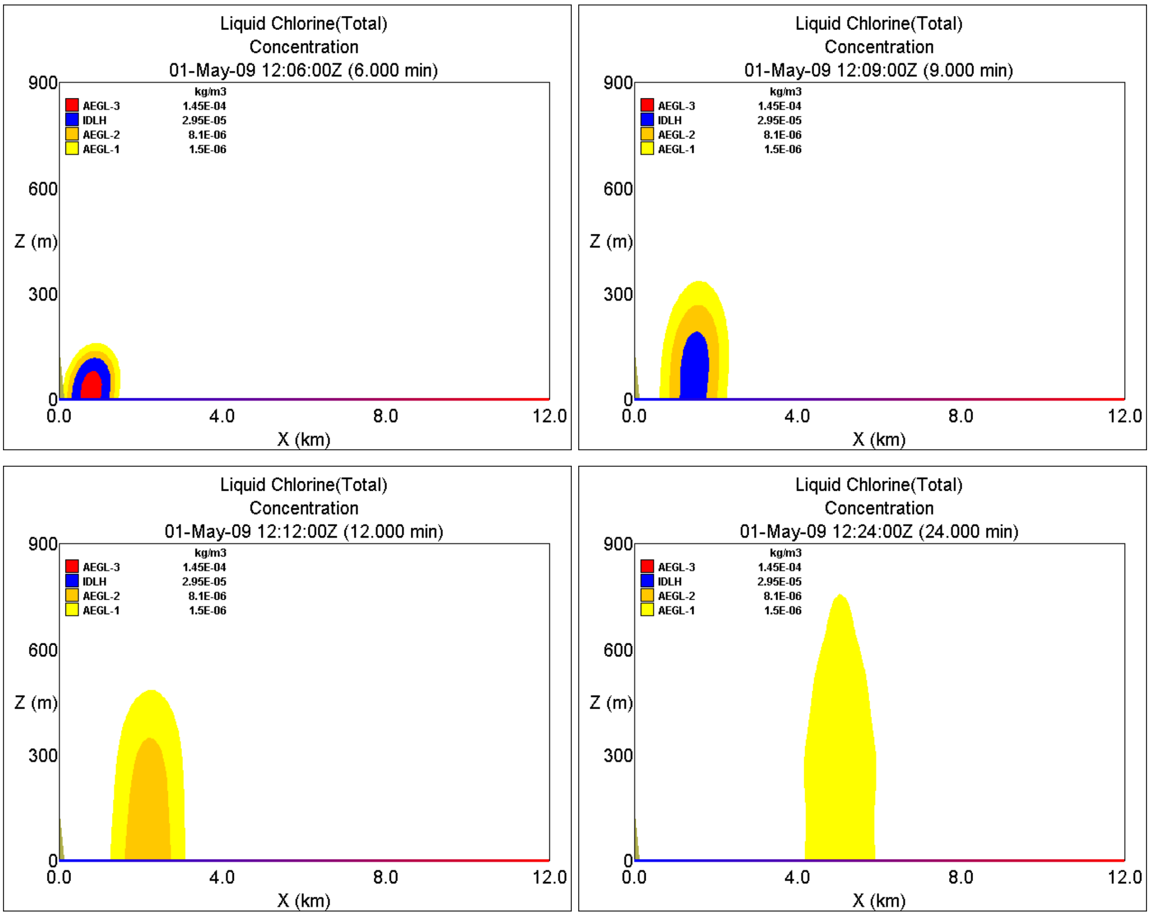

Figure 4.6 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC (fixed wind module). The wind speed is 3 m/s from west. The plots show the vertical concentration profiles downwind from the release at which the AEGL-3 concentration level persists (6 min) (upper left) and the same situation for the IDLH level (9 min) (upper right), for AEGL-2 level (12 min) (lower left) and for the AEGL-1 level (24 min) (lower right).

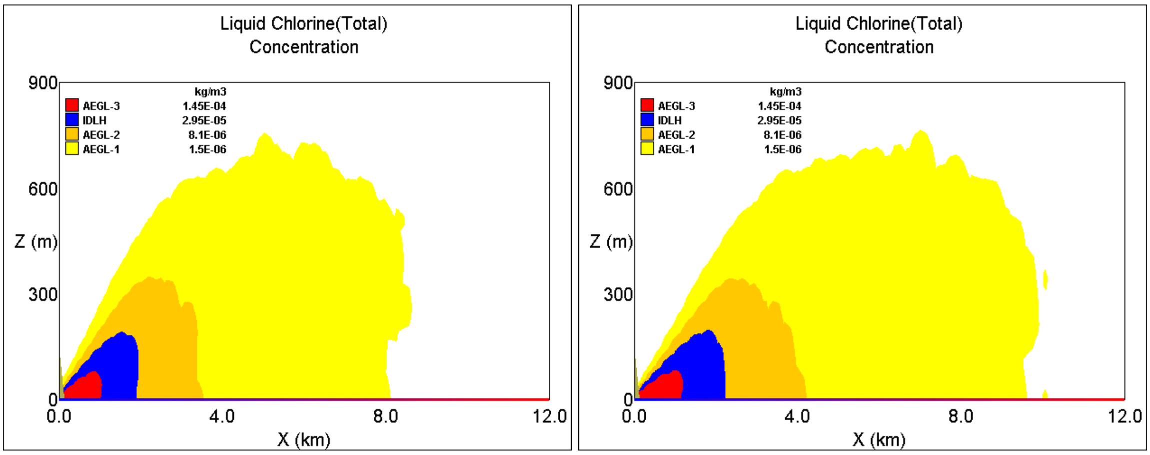

Figure 4.7 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC for wind speed 3 m/s from west. The plot represents the maximum vertical downwind areas affected by the threshold concentrations (AEGL-1, AEGL-2, IDLH and AEGL-3) for the fixed wind weather module (HPAC-1)(left) and the manual weather module (HPAC-2)(right).

In Figure 4.8, the horizontal chlorine profiles predicted by ARGOS are shown. The screen shots are taken at the times when the concentration in the plume drops below the AEGL-3, IDLH, AEGL-2 and AEGL-1 levels. Note that the concentration levels in the figure is shown with black lines and that the coloured gas plume are larger than represented by the actual concentration limits.

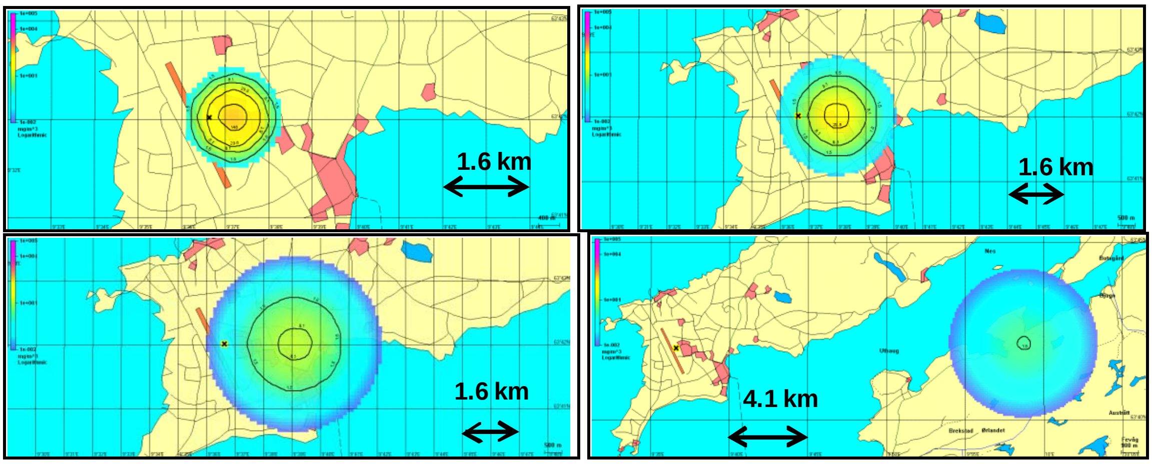

Figure 4.8   Release of 6000 kg chlorine at Ørland MAS modelled by ARGOS for wind speed 3 m/s from west. The plots represent the time when the concentrations drop below the AEGL-3 level (4 min) (upper left), IDLH level (7 min) (upper right), AEGL-2 level (10 min) (lower left) and AEGL-1 level (78 min) (lower right), respectively.

In Figure 4.9, the total area affected by the specified concentration level is shown. Note that this figure does not show the concentration variation with time and that the whole area will not be affected simultaneously.

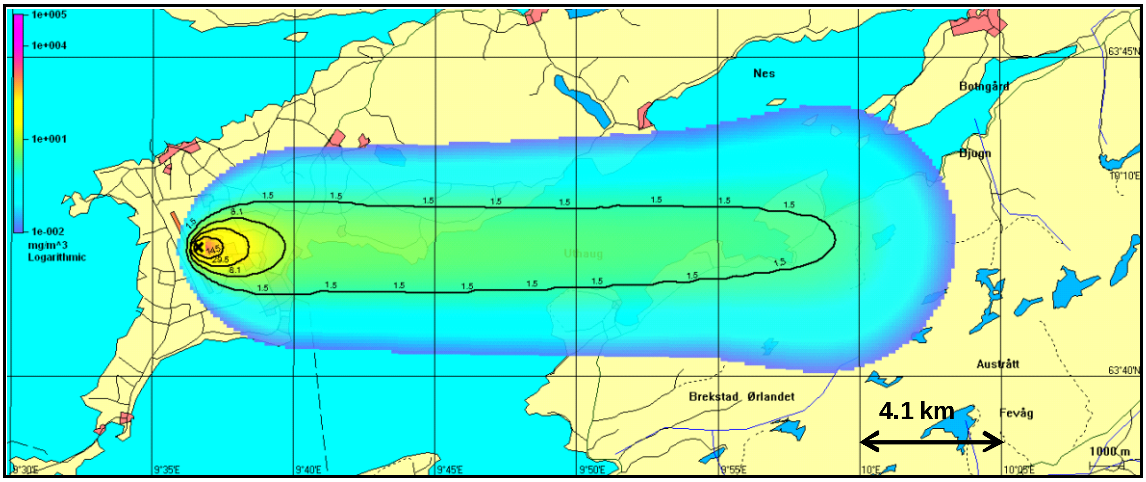

Figure 4.9   Release of 6000 kg chlorine at Ørland MAS modelled by ARGOS for wind speed 3 m/s from west. The black lines encompass the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3).

Vignette 2: Wind from 225 degrees (over land)

In this vignette, the wind direction was from south-west (225°), and the plume will travel only above land. The plots from HPAC are shown in Figure 4.10, from ARGOS in Figure 4.11, and from DEGADIS in Figure 4.12.

In Figure 4.10 and Figure 4.11, the total areas affected by the specified concentration level are shown. Note that these figures do not show the concentration variations with time and that the whole area will not be affected simultaneously.

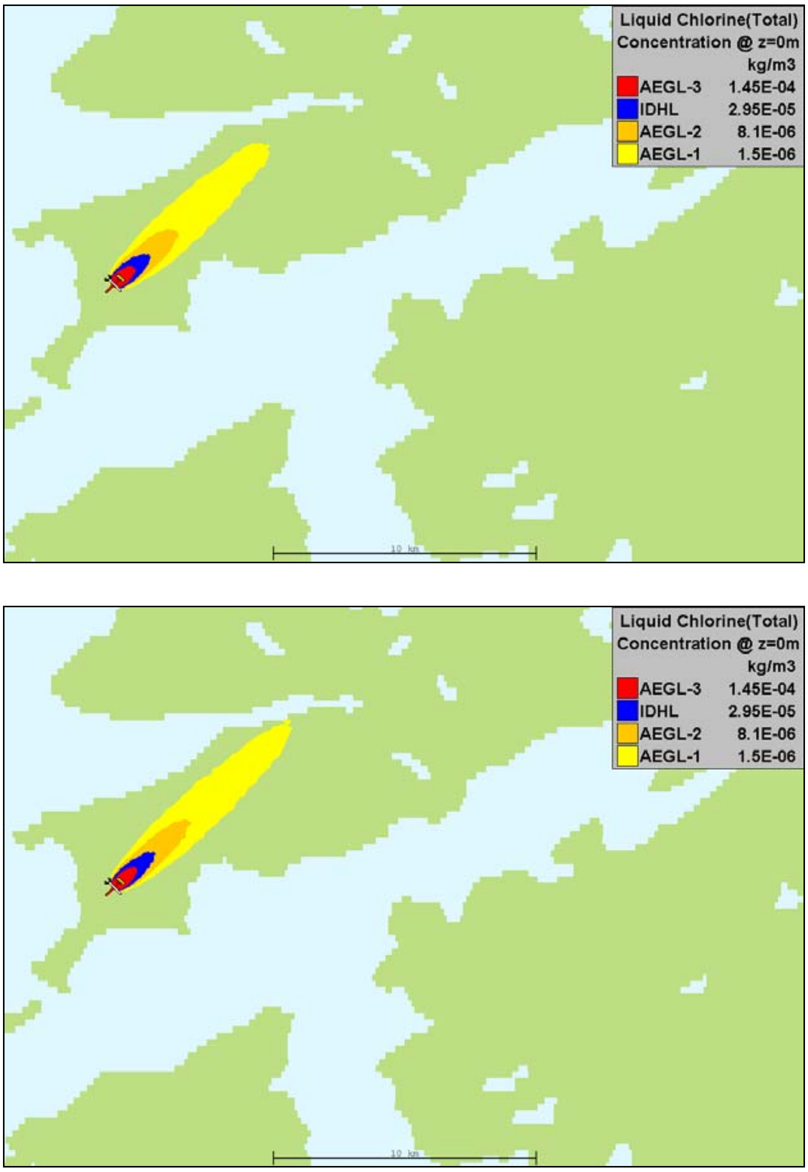

Figure 4.10 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC for wind speed 3 m/s from south-west (225°). The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3) for the fixed wind weather module (HPAC-1)(top) and the manual weather module (HPAC-2)(bottom).

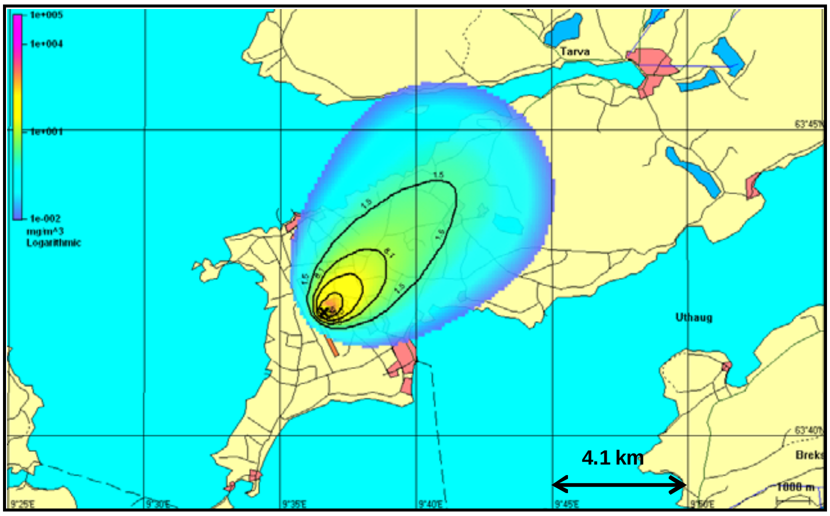

Figure 4.11 *Release of 6000 kg chlorine at Ørland MAS modelled by ARGOS for wind speed 3 m/s from south-west (225°). The black lines encompass the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3).*

The DEGADIS program does not take the surface into consideration except for the roughness parameter. DEGADIS simulations are conducted for a surface roughness of 0.1 m, corresponding to grassland [12]. The plume at the time steps where the concentration drops below AEGL-3, IDLH, AEGL-2 and AEGL-1 levels, respectively, is shown in Figure 4.12. Since DEGADIS does not produce a graphic result file directly, these figures were created with MATLAB.

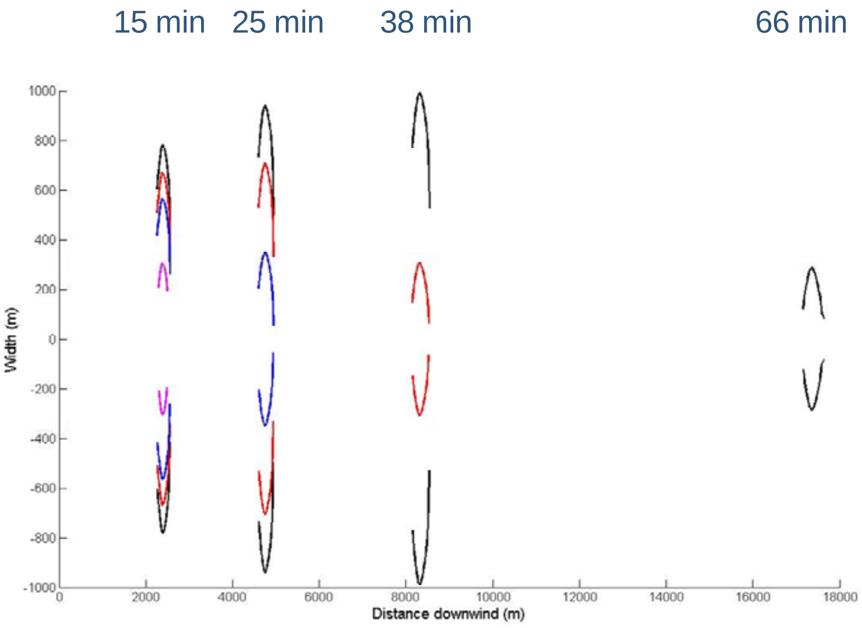

Figure 4.12 *Release of 6000 kg chlorine at Ørland MAS modelled by DEGADIS for wind speed 3 m/s from south-west (225°) and dispersion above land. The figure shows the widths of the clouds containing concentrations corresponding to AEGL-1 (black line), AEGL-2 (red line), IDLH (blue line) and AEGL-3 (purple line). The plots show the situations when the concentrations drop below AEGL-3 (15 minutes), IDLH (25 minutes), AEGL-2 (38 minutes) and AEGL-1 (66 minutes), respectively (from left to right).*

In this vignette (with wind from south-west), we also looked at the concentration profile close to the ground perpendicular to the wind direction 500 m downwind from the release point (Figure 4.13, left). In this way we can see the width of the plume close to the ground. The concentrations for DEGADIS are taken at a height of 1.6 m above ground. In Figure 4.13 (right), the vertical concentration profiles at centreline 500 m downwind from the release point from HPAC and DEGADIS are shown. A similar plot from ARGOS is not easily available.

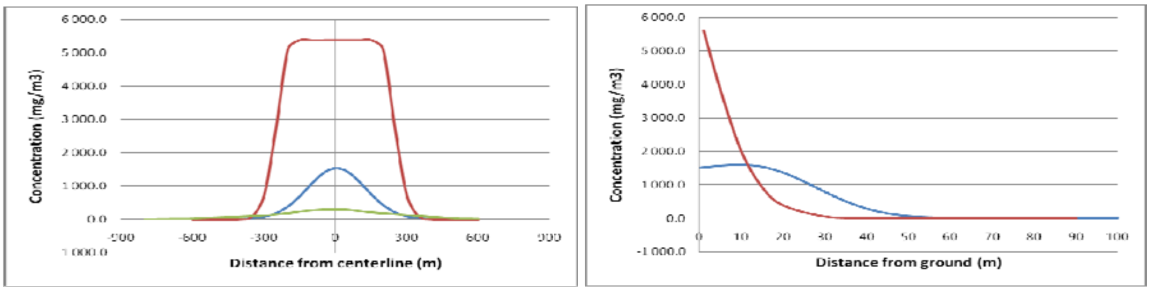

Figure 4.13 Chlorine concentration profiles in the left figure are obtained 500 m downwind from the release, perpendicular to the wind direction (wind from south-west). The figure at right shows the vertical concentration profiles at centreline 500 m downwind from the release. Colour codes; DEGADIS (red), HPAC (blue) and ARGOS (green).

As can be seen from these figures, the concentrations predicted by DEGADIS have a steeper rise when moving from a point outside the affected area and in towards the centerline than the concentration profile predicted by HPAC and ARGOS. At 500 m downwind from the source, DEGADIS predicts the highest concentration and ARGOS the lowest concentrations.

When looking at the vertical concentration profile of the chlorine plume using DEGADIS and HPAC Figure 4.13 (right), it is apparent that DEGADIS predicts a more concentrated plume which does not reach the same height as the plume predicted by HPAC. HPAC gives, on the other hand, a less dense cloud which reaches higher above ground.

Vignette 3: Wind from 90° (over sea)

In this vignette, the wind direction was chosen from east (90°), where the plume will travel mostly over sea. The plots from HPAC are shown in Figure 4.14, from ARGOS in Figure 4.15 and from DEGADIS in Figure 4.16.

In Figure 4.14 and Figure 4.15, the total areas affected by the specified concentration level are shown. Note that this figure does not show that the concentration varies with time and that the whole area will not be affected simultaneously.

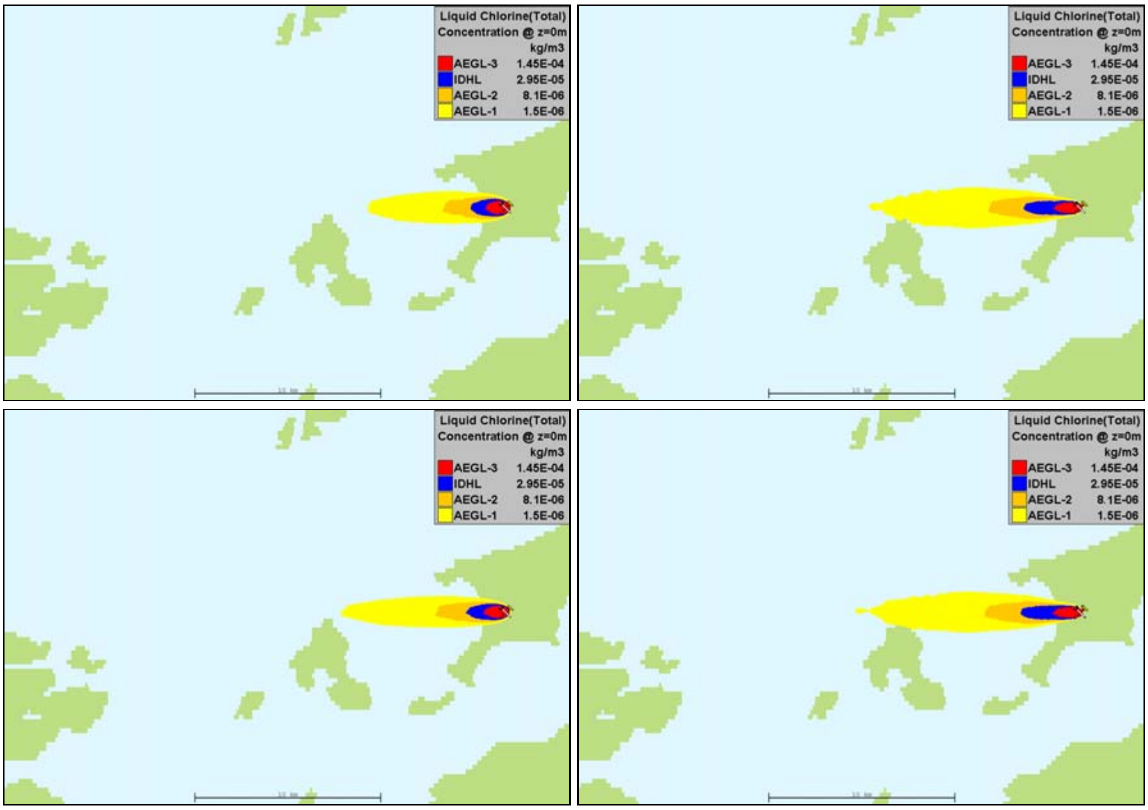

Figure 4.14 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC for wind speed 3 m/s from east. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3) for the fixed wind weather module (HPAC-1) upper and the manual weather module (HPAC-2) lower. The left plots show the affected area when using grassland, the right plots showing the affected area when using water.

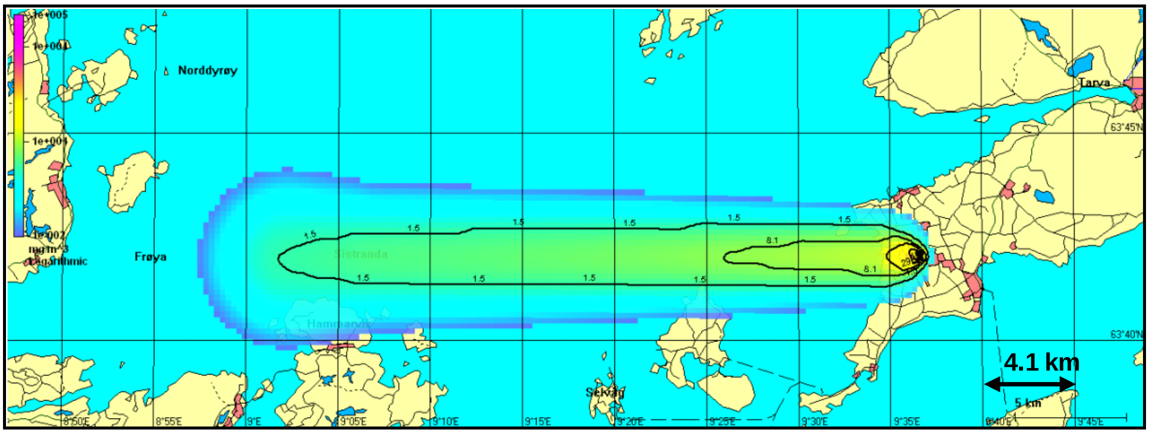

Figure 4.15 Release of 6000 kg chlorine at Ørland MAS modelled by ARGOS for wind speed 3 m/s from east. The black lines in the plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3).

DEGADIS simulations are conducted for a surface roughness of 0.0005 m, corresponding to water [12]. The plume at the time steps where the concentration drops below AEGL-3, IDLH, AEGL-2 and AEGL-1 levels, respectively, is shown in Figure 4.16.

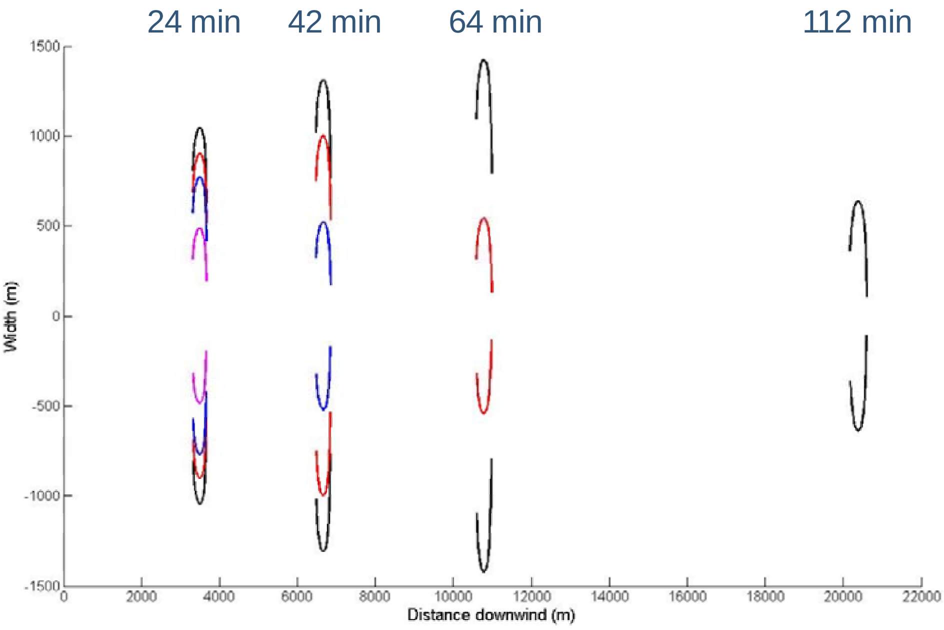

Figure 4.16 Release of 6000 kg chlorine at Ørland MAS modelled by DEGADIS for wind speed 3 m/s, and dispersion above sea. The figure shows the widths of the plume containing concentrations corresponding to AEGL-1 (black line), AEGL-2 (red line), IDLH (blue line) and AEGL-3 (purple line). The plots show the situations when the concentrations drop below the AEGL-3 (24 minutes), IDLH (42 minutes), AEGL-2 (64 minutes) and AEGL-1 (112 minutes), respectively (from left to right).

4.4.2 Discussion

In this scenario, the only difference in the three vignettes are the land cover (surface) over which the plume travels. The maximum distances that the chlorine plumes travel and the maximum plume widths with the corresponding travel times are given in Table 4.4 for all three vignettes. In addition, the height of the plume, calculated by HPAC, is shown for each run.

Wind from (degree)	Software	Concentration limit	Max distance (km)	Max width (km)	Max height of plume (m)
270[1]	HPAC-1 Fixed wind	AEGL-1	8.1 (36 min)	1.8 (17min)	760 (24 min)
		AEGL-2	3.1 (16 min)	1.1 (9 min)	350 (12 min)
		IDLH	1.9 (10 min)	0.8 (6 min)	190 (9 min)
		AEGL-3	1.0 (6 min)	0.6 (4 min)	80 (6 min)
270[1]	HPAC-2 Manual weather	AEGL-1	9.6 (36 min)	1.8 (17 min)	760 (28 min)
		AEGL-2	3.9 (16 min)	1.0 (9 min)	340 (11 min)
		IDLH	2.2 (10 min)	0.8 (6 min)	195 (9 min)
		AEGL-3	1.1 (6 min)	0.6 (4 min)	80 (6 min)
270[1]	ARGOS	AEGL-1	19 (78 min)	2.7 (11 min)	NA
		AEGL-2	2.1 (10 min)	1.7 (5 min)	NA
		IDLH	1.3 (7 min)	1.0 (3 min)	NA
		AEGL-3	0.5 (4 min)	0.6 (2 min)	NA
225[2]	HPAC-1 Fixed wind	AEGL-1	8.2 (36 min)	1.8 (17 min)	730 (24 min)
		AEGL-2	3.2 (16 min)	1.1 (9 min)	345 (12 min)
		IDLH	1.8 (10 min)	0.8 (6 min)	190 (9 min)
		AEGL-3	1.0 (6 min)	0.6 (4 min)	75 (6 min)
225[2]	HPAC-2 Manual weather	AEGL-1	9.7 (36 min)	1.7 (17 min)	740 (24 min)
		AEGL-2	4.0 (16 min)	1.0 (9 min)	345 (11 min)
		IDLH	2.1 (10 min)	0.8 (6 min)	195 (9 min)
		AEGL-3	1.1 (6 min)	0.5 (4 min)	80 (6 min)
225[2]	ARGOS	AEGL-1	5.3 (24 min)	2.7 (11 min)	NA
		AEGL-2	2.3 (11 min)	1.6 (5 min)	NA
		IDLH	1.3 (7 min)	1.1 (4 min)	NA
		AEGL-3	0.6 (4 min)	0.6 (2 min)	NA
225[2]	DEGADIS	AEGL-1	18 (66 min)	2.0 (36 min)	NA
		AEGL-2	8.5 (38 min)	1.4 (22 min)	NA
		IDLH	4.9 (25 min)	1.1 (15 min)	NA
		AEGL-3	2.5 (15 min)	0.9 (10 min)	NA
90[3]	HPAC-1 Fixed Wind	AEGL-1	11 (58 min)	2.5 (31 min)	445 (33 min)
		AEGL-2	5.0 (26 min)	1.4 (16 min)	250 (18 min)
		IDLH	3.1 (16 min)	0.9 (7 min)	160 (12 min)
		AEGL-3	1.5 (9 min)	0.6 (4 min)	75 (8 min)
90[3]	HPAC-2 Manual Weather	AEGL-1	12 (58 min)	2.4 (29 min)	435 (28 min)
		AEGL-2	5.4 (27 min)	1.4 (16 min)	250 (18 min)
		IDLH	3.2 (16 min)	0.9 (7 min)	155 (12 min)
		AEGL-3	1.6 (9 min)	0.6 (4 min)	75 (8 min)
90[3]	ARGOS	AEGL-1	28 (112 min)	2.7 (10 min)	NA
		AEGL-2	8.8 (36 min)	1.7 (6 min)	NA
		IDLH	1.3 (7 min)	1.0 (4 min)	NA
		AEGL-3	0.5 (3 min)	0.5 (3 min)	NA
90[3]	DEGADIS	AEGL-1	21 (112 min)	2.8 (66 min)	NA
		AEGL-2	11 (64 min)	2.0 (40 min)	NA
		IDLH	6.8 (42 min)	1.6 (28 min)	NA
		AEGL-3	3.7 (24 min)	1.1 (18 min)	NA

Table 4.4 Maximum plume travel distance, width and height at given concentration limits.
[1] Wind direction from west (270°) - including terrain information
[2] wind direction from south-west (225°) - terrain is only land
[3] wind direction from east (90°) - terrain is only sea
NA: Not applicable

The maximum distance the plume travels before the concentration drops below the concentration limits AEGL-1, AEGL-2, IDLH and AEGL-3 in the three vignettes are shown in Figure 4.17.

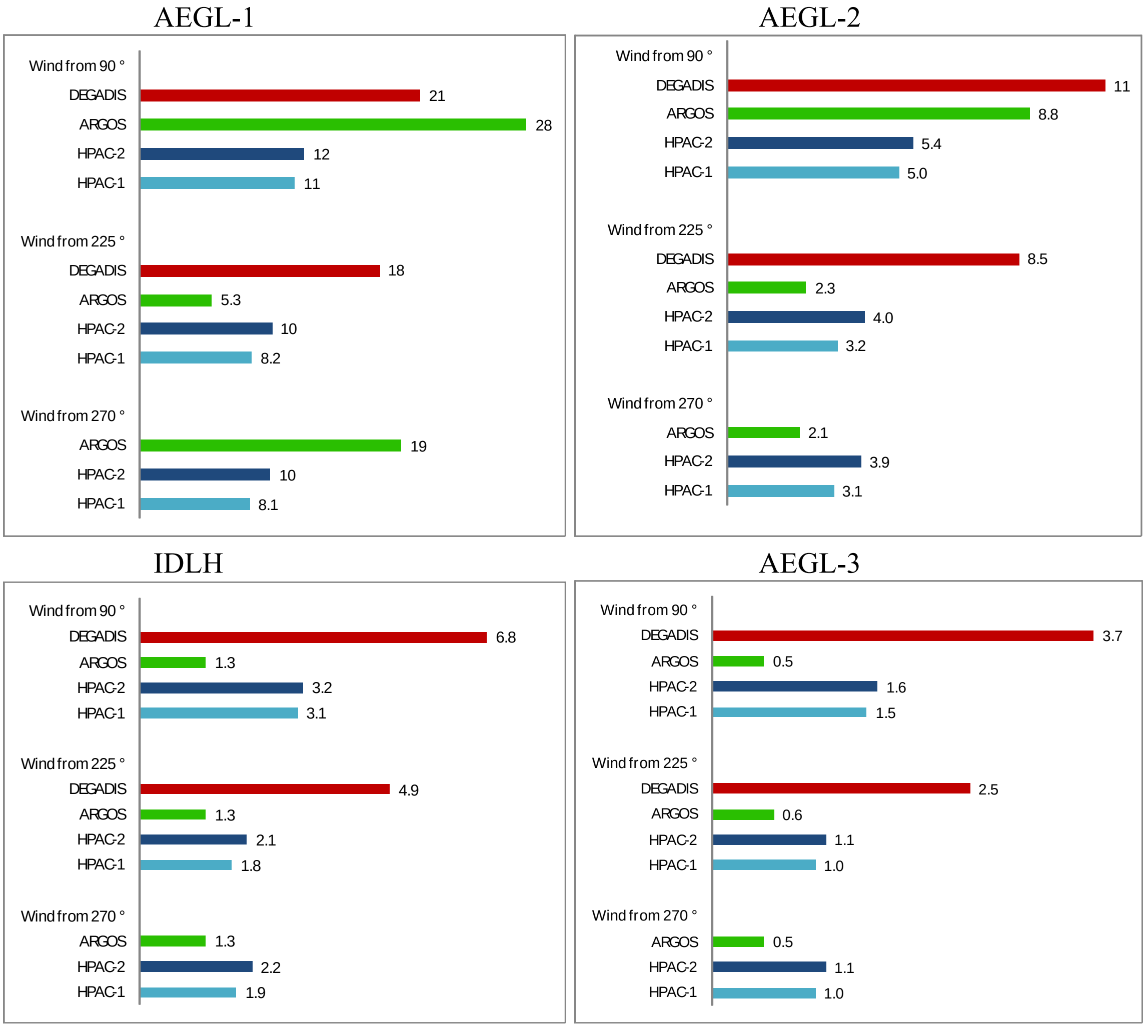

Figure 4.17 Maximum distance (in km) the chlorine plume travel before the concentration drops below the concentration limits AEGL-1 (top left), AEGL-2 (top right), IDLH (bottom left) and AEGL-3 (bottom right) for the three vignettes.

The differences between the results from “fixed wind” (HPAC-1) and “manual weather” (HPAC-2) for HPAC are small. The maximum distances that the plume travel before the concentration drops below the concentration limits are generally slightly larger with use of “manual weather” (HPAC-2). The reason for this is that the fixed wind mode uses a reference height of 10 m for the given input, whereas 5 m is used for the manual weather mode and consequently the wind speed close to the ground will be higher for the manual weather runs.

As can be seen from Figure 4.17, HPAC gives similar results for wind directions from 270° and 225°. The reason for this is that the land cover option was not used and consequently the calculation domain was assumed to have the same surface across the calculation domain. With wind from 90°, the surface was changed from grassland to water to identify the effect of the land cover on the distribution calculation. The results here are therefore different from the other wind directions (see also Figure 4.14).

In contrast, the results from ARGOS are very dependent on the terrain data, especially for the lower concentration limit (AEGL-1). The maximum distances that the plume travel before the concentration drops below AEGL-1 varies from 5.3 km over land (which is lower than the results from HPAC) to 19.2 km with combined land and sea cover to 28.4 km over sea (both much larger than the results from HPAC). For the AEGL-2 limit, the variations are much smaller (2.2 km, 2.2 km and 8.0 km) and for the IDLH and AEGL-3 limits, the travelled distances are almost equal.

The wind turbulence determines how fast the chemical puffs mix with air when they travel downwind from the release. Over water, the surface roughness is very low (see Table 2.3) and the plume will mix very slowly compared to when it travels over land. If the surface temperature is less than the air (e.g. over water), the atmosphere will be stable and the plume can travel longer distances over sea as compared to land.

ARGOS show large differences at the lowest concentrations (AEGL-1) level, but almost no differences at the higher concentration limits (IDLH and AEGL-3 levels). The reason for this might be that the surface is land in all directions close to the release point and the concentration drops below the concentration limits before the plume reaches the sea.

From Figure 4.17 we also see that the predicted distance the cloud travels before the concentration drops below the given limits generally are largest for the DEGADIS results, except with wind from east (90°) at the AEGL-1 level, where ARGOS gives the longest travel distance. The difference between HPAC-1 and HPAC-2 are small. The distances the chlorine plume will travel before it drops below the IDLH and AEGL-3 limits are generally lower calculated with ARGOS than with HPAC.

The results from ERGO (PAD = 3.5 km) is in this scenario similar to what is obtained for IDLH or AEGL-2 limits from HPAC and ARGOS. The result from DSB ”Farlig gods” (484 m) is similar to the AEGL-3 level from HPAC and ARGOS. The DSB ”Farlig gods” gives results that are meant to describe concentrations which could give life-threatening effects or death.

4.5 Meteorological data from radiosonde

4.5.1 Dispersion modelling and simulation

In this scenario, the meteorological data was obtained from a radiosonde at Ørland MAS at two different heights above ground (Table 4.5). For DEGADIS it is only possible to enter wind data in one height, and DEGADIS results are therefore not included in this comparison. Since version 8.3 of ARGOS only can handle correctly readings from two different heights, the readings from 7 m and 130 m were used[13]. The radiosonde readings from Ørland at 1100 UTC on 19 May 2009 are given in Table 4.5 below. The wind is from west, and the terrain in this case is both land and sea.

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[13] Radiosonde data from 7 m and upward are available from Ørland

Other input parameters are given in Table 4.6. In HPAC, the release was defined using the analytic module.

Pressure (mbar)	Height above ground (m)	Temp (°C)	Dew point (°C)	Wind from (Degrees)	Wind speed (m/s)
1014.0	7	14.2	6.2	270	5.0
1000.0	130	12.0	6.0	275	4.0

Table 4.5 Meteorological conditions at Ørland 19 May 2009 at 1100Z.

Input parameter	Value	HPAC	ARGOS
Released gas	Chlorine	X[3)]	X
Released amount	6000 kg - vapour	X	X
Release rate	100 kg/s (60 sec)	X	X
Surface roughness		Grassland (0.1 m)	From map
Cloud cover (octavos)[1)]	Overcast (8)	X	X
Precipitation (mm)	0	X	X
Relative humidity (RH)	60 % [2)]	X	X
Date	19.05.2009 at 1100Z	X	X
Release height (above ground)		2 m	Ground level
Sampling height		Surface	Surface

Table 4.6 Input parameters.

[1)] Cloud cover is measured in octavos (1-8, and 0=clear sky)

[2)] Relative humidity calculated from temperature and dew point in Table 4.5

[3)] X: Used by the program

The results from the simulations are shown in Table 4.7 and in Figure 4.18 and Figure 4.19. The table shows the maximum distance downwind and the maximum widths calculated with HPAC and ARGOS, and also the maximum height of the plume calculated with HPAC. The figures show the maximum area affected horizontally (HPAC and ARGOS) and also vertically (HPAC).

Software	Concentration limit	Max distance (km)	Max width (km)	Max height of plume (m)
HPAC	AEGL-1	11 (35 min)	1.7 (12 min)	745 (22 min)
	AEGL-2	4.5 (15 min)	1.0 (8 min)	365 (11 min)
	IDLH	2.5 (9 min)	0.7 (5 min)	200 (8 min)
	AEGL-3	1.3 (6 min)	0.5 (4 min)	90 (5 min)
ARGOS	AEGL-1	14 (47 min)	2.8 (11 min)	NA
	AEGL-2	2.4 (8 min)	1.7 (5 min)	NA
	IDLH	1.4 (5 min)	1.0 (3 min)	NA
	AEGL-3	0.5 (2 min)	0.5 (2 min)	NA

Table 4.7 The maximum distance the chlorine plume travel and the maximum plume width and plume height at different concentration limits using HPAC and ARGOS
NA: Not applicable.

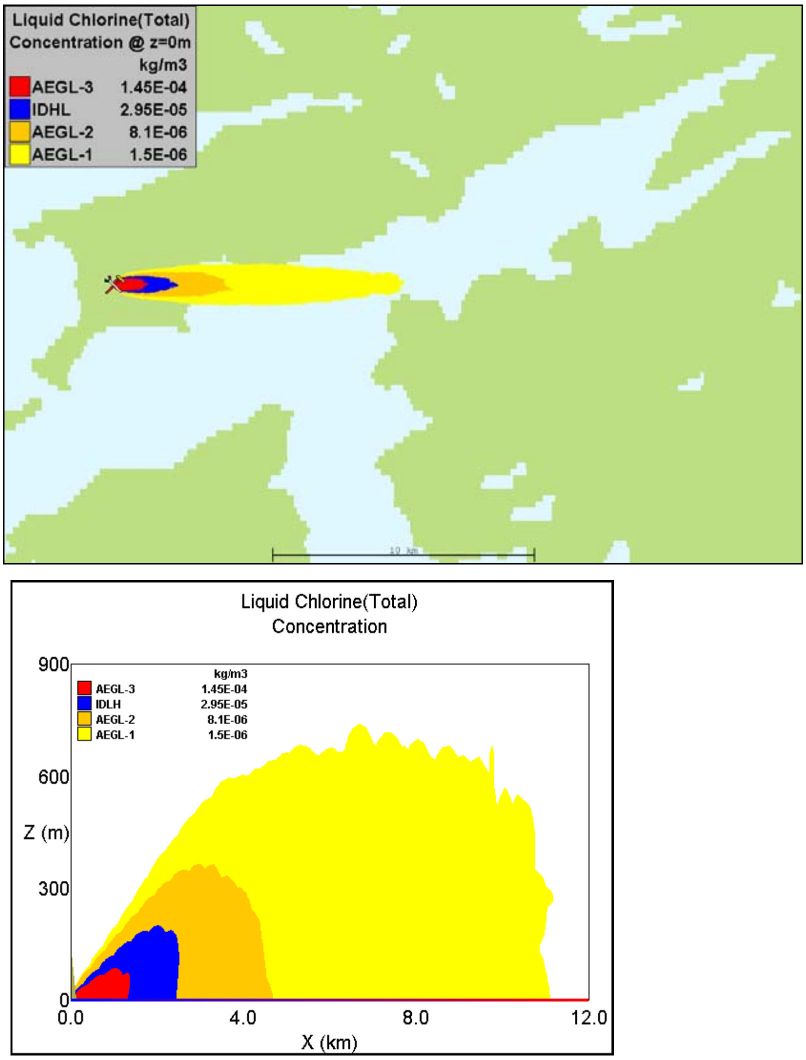


Figure 4.18 Release of 6000 kg chlorine at Ørland MAS modelled by HPAC. Meteorological data from a radiosonde at 19 May 2009 has been used. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3) for the horizontal plane (top) and the vertical downwind plane (bottom).

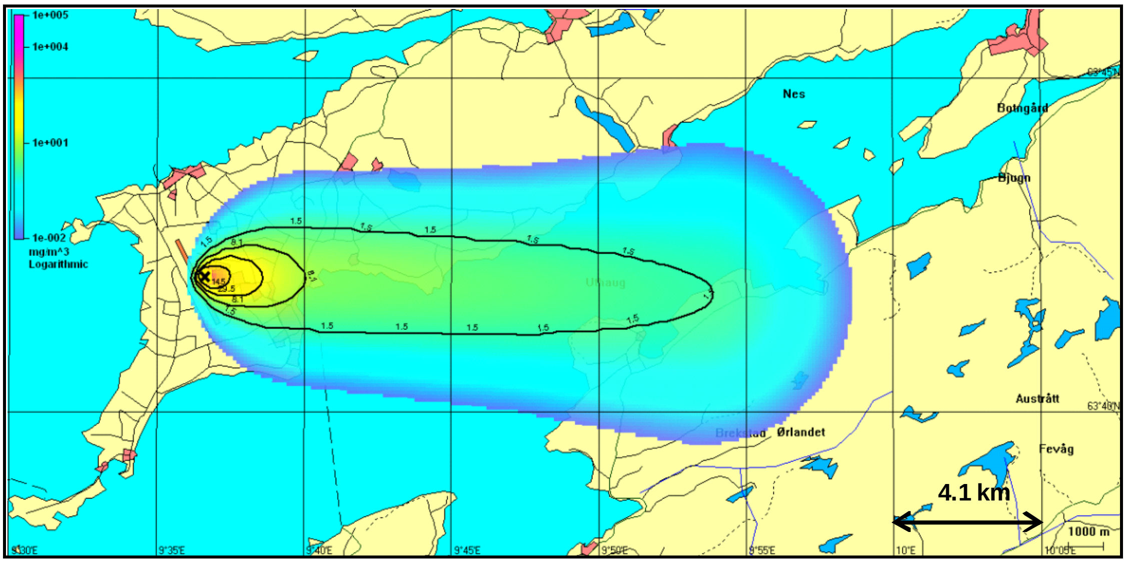


Figure 4.19 Release of 6000 kg chlorine at Ørland MAS modelled by ARGOS. Meteorological data from a radiosonde at 19 May 2009 has been used. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3).

4.5.2 Discussion

In this scenario, the differences between the results from HPAC and ARGOS are not so large. Again, ARGOS gives larger maximum travelled distance for the lowest concentration limit (AEGL-1), but smaller distances for AEGL-2, IDLH and AEGL-3.
It should be noted that the meteorological conditions are different in this scenario compared to the previous ones (Chapter 4.4). As an example, the wind speed is 5 m/s at ground level in this scenario, compared to 3 m/s in the previous one. The results are therefore not comparable. It is therefore not known if the weather obtained at two different heights have any effect on the results. This simulation was, however, carried out as an example on what the programs can handle.

4.6 Release of chlorine including source modelling

ARGOS and HPAC have dedicated source modelling tools (see chapter 2.4) which were of interest to test and compare with the pool evaporation model in the TNO Yellow Book, which in this work is used as input to DEGADIS.

4.6.1 Release

The input parameters for this release are taken from a scenario constructed in the course of a European Defence Agency project [1]. A tanker (truck) with chlorine is fitted with explosives and a timer, abandoned outside the camp at Ørland MAS, and the explosives then set off. The temperature during the release was 14.2 °C. Input parameters for the chlorine release are shown in Table 4.2.

During such a release, a fraction of the liquid evaporates immediately (flashing), some liquid is dispersed as aerosols (airborne droplets), while the rest of the liquid forms an evaporating pool on the ground. Explanation of the calculations performed to obtain the amount of mass that is airborne and also the evaporation rate from the pool is given in Chapter 3.

4.6.2 Dispersion modelling

We have used the same meteorological conditions (19 May 2009) for this release as in Chapter 4.5 above (see Table 4.5). The surface under the pool is assumed to be dry sand and the surface of the environment outside the pool is assumed to be grass land. The maximum travel distance before the concentration in the plume is below the concentration limits are given in Table 4.8 below, together with the duration of the plume above the release site and the maximum height of the plume, if available.

Program	Evaporation rate at 1 min (kg/s)	Concentration limit	Max distance (km)	Duration of concentration above limit at release site (min)	Max height of plume (m)
HPAC	36.4	AEGL-1	16	11	900
		AEGL-2	6.6	11	470
		IDLH	3.7	11	270
		AEGL-3	1.6	11	110
ARGOS	32.6	AEGL-1	19	66	NA
		AEGL-2	6.6	25	NA
		IDLH	2.0	24	NA
		AEGL-3	0.9	12	NA
DEGADIS	19.8	AEGL-1	23	NA	NA
		AEGL-2	11	NA	NA
		IDLH	6.4	NA	NA
		AEGL-3	2.2	NA	NA

Table 4.8 Duration of the chlorine cloud at release site and maximum distance and height of the plume predicted by HPAC, ARGOS and DEGADIS after release at Ørland MAS when the source modelling is included.
NA: Not applicable

Figure 4.20 shows the areas affected by the concentration levels AEGL-1, AEGL-2, IDLH and AEGL-3 in the horizontal and vertical plane, calculated with HPAC. Figure 4.21 shows the maximum areas affected in the horizontal plane calculated with ARGOS.

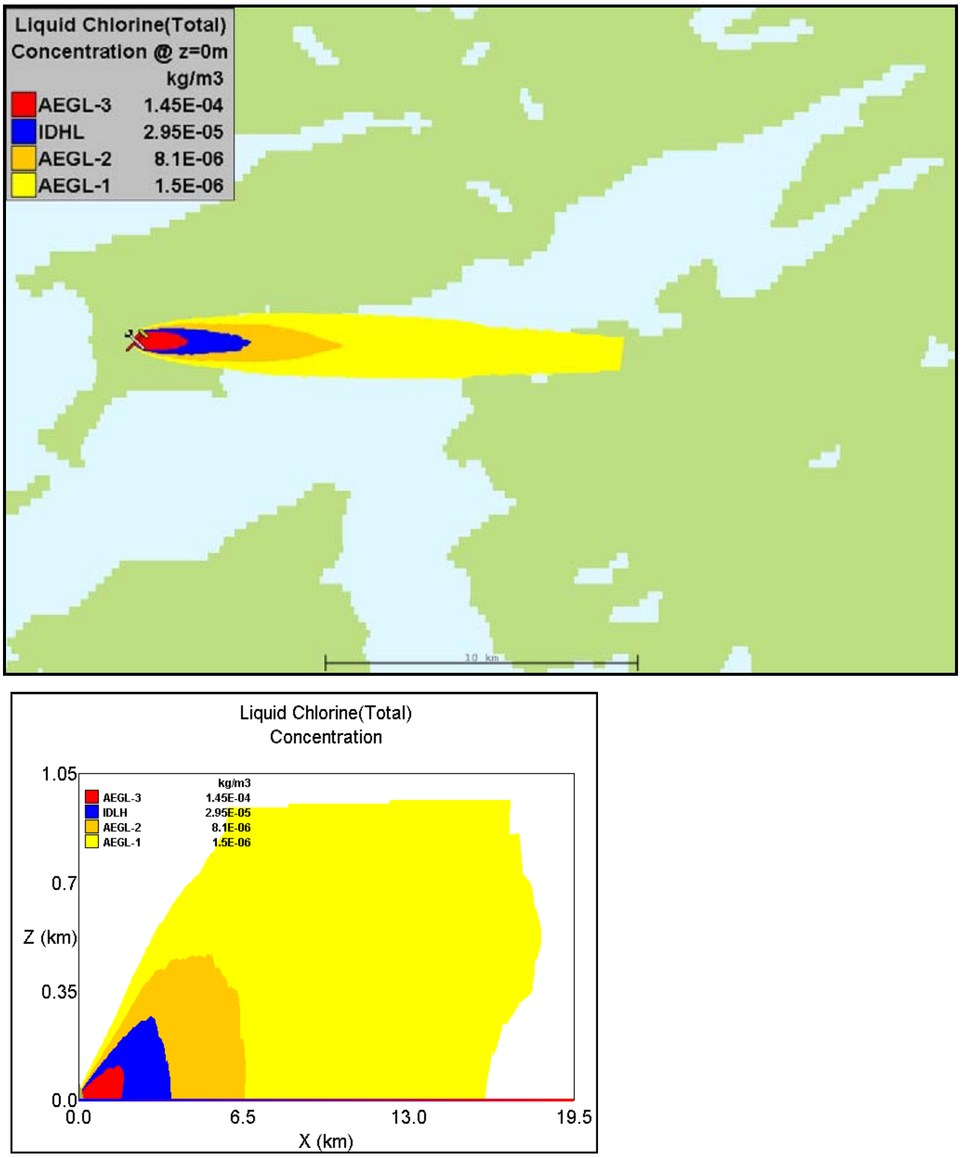


Figure 4.20 Release of 20 tons of chlorine at Ørland MAS modelled by HPAC (6 tons as gas and 14 tons as liquid). The liquid evaporates during 11 min. The wind speed is 5 m/s from 270° at 7 m height. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3) for the horizontal plane to the left and the vertical downwind plane to the right.

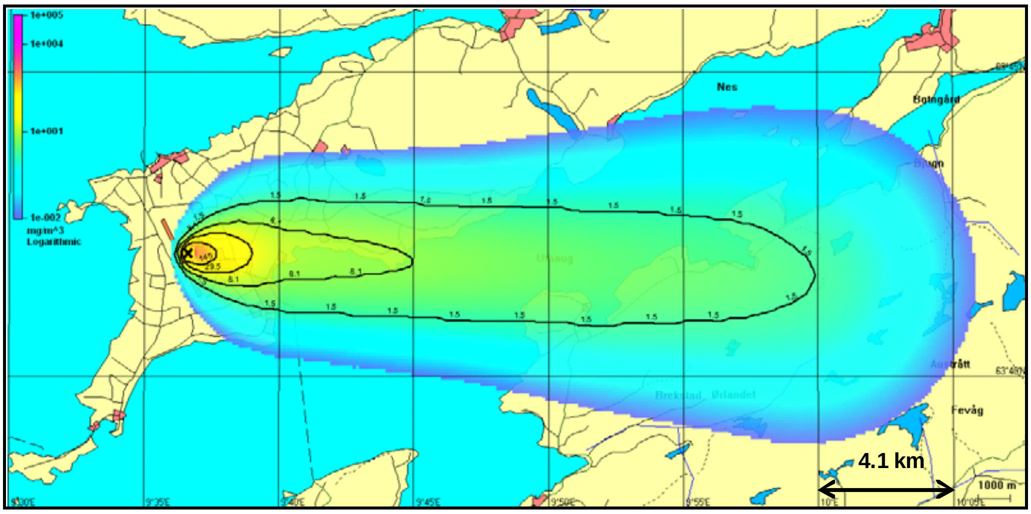


Figure 4.21 Release of 20 tons of chlorine at Ørland MAS modelled by DEGADIS (6 tons as gas and 14 tons as liquid). The liquid evaporates during 23 min. The wind speed is 5 m/s from 270° at 7 m height. The black lines in the plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3).

4.6.3 Discussion

The dispersion process can in this case be divided in two phases: first, an initial plume (corresponding to the simulations in Chapter 4.4.1); and secondly, a plume created by the evaporating pool (Chapter 4.6.1). The initial plume caused by flashing (seconds) will be more massive than the secondary plume from the evaporation process which lasts much longer (min – hours). Depending on the evaporation rate, the secondary evaporation process can affect the size of the hazard area in a larger or smaller degree. It will also affect the area relatively close to the pool by prolonging the time of hazard.

The initial concentration of chlorine in the air after the release is different for the different models. The evaporation rate after one minute for HPAC and ARGOS is about twice the rate obtained by the Yellow Book procedure (Figure 3.3). The duration of the plume above the release site is much longer for ARGOS as compared to HPAC, see Table 4.8. This information is not easily available from DEGADIS, but it is strongly related to the evaporation rate calculated with the Yellow Book formulas.

The fact that a much slower pool evaporation process is given as input to DEGADIS does not explain why DEGADIS gives longer hazard distances downwind than HPAC and ARGOS. The reason for this is similar for all the chlorine scenarios and might be because DEGADIS is a model designed to handle dense gases (like chlorine) and therefore predicts a plume which is more concentrated close to the ground (due to gravity effects) and is dispersed for a longer distance downwind. HPAC and ARGOS, which have similar evaporation rates, also give similar maximum downwind distances for the predicted concentration (Figure 4.20 and Figure 4.21). The plume reaches somewhat further in the downwind direction when the pool evaporation process is included (compare Table 4.8 with Table 4.4). It is clearly seen that the hazard prevail for a much longer time in the ARGOS simulation than HPAC, reflecting the lower evaporation rate and correspondingly longer duration of the evaporation process in the ARGOS simulation.

Also in this scenario (Figure 4.22), ARGOS gives a longer maximum travel distance downwind than HPAC for the AEGL-1 level, while the distances for the higher concentration levels are smaller with ARGOS than HPAC. DEGADIS predicts the longest maximum travel distance downwind in agreement with the preceding simulations.

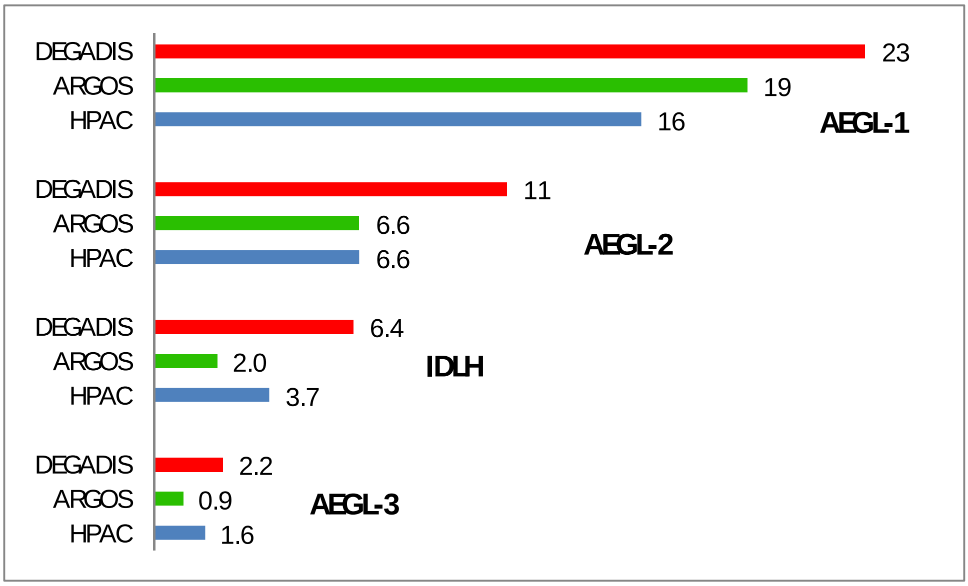


Figure 4.22 Maximum distance (in km) the chlorine plume travels before the concentration drops below the concentration limits AEGL-1, AEGL-2, IDLH and AEGL-3 for the release including pool evaporation described in the text.

5 Modelling and simulation results for ammonia release

5.1 Scenario description

In this scenario, ammonia is released from a ruptured tanker close to Kjeller. The tanker contains 10 000 kg liquefied ammonia which is released in one minute. In these simulations we include the source modelling part directly (and do not look at gas phase only). The simulations are carried out at three different times of the year with three different meteorological conditions (vignettes 1-3).

The toxicological limits for ammonia (calculated for an exposure time of 10 min) are, AEGL-1 = 21.0 mg/m^3, AEGL-2 = 154 mg/m^3, IDLH = 210 mg/m^3, AEGL-3 = 1898 mg/m^3[25;26]. The input parameters are given in Table 5.1.

Parameter	Value
Time of day	0600Z
Position (MGRS)	32VPM 1410650030
Compound released	Ammonia
Amount released (total)	10 000 kg
Released as gas and aerosol	See Table 5.2
Released as liquid	See Table 5.2
Toxicological limits	
AEGL-1	21.0 mg/m^3 [25]
AEGL-2	154 mg/m^3 [25]
IDLH	210 mg/m^3 [26]
AEGL-3	1898 mg/m^3 [25]

Table 5.1 Input parameters.

The flash fraction, the mass of the initial airborne plume and the mass and area of the pool on the ground calculated as described in Chapter 3.1 are given in Table 5.2.

Vignette	Temp. (ºC)	Wind speed (m/s)	Vapour mass fraction (from flashing)	Mass of initial cloud (gas + aerosols) (kg)	Mass of pool (kg)	Area (m^2)
1	-15	2.0	0.06	1200	8800	1290
2	14	6.4	0.15	3000	7000	1026
3	6	8.9	0.12	2400	7600	1114

Table 5.2 Ammonia release characteristics.

The surface under the pool is defined as asphalt, and the surface of the environment in the rest of the area is defined as grass land with a surface roughness of 0.1 m. It is assumed that the depth of the pool will be 1 cm (this corresponds to normal sandy soil, gravel, railroad yard according to the TNO Yellow Book [22][14]).

The evaporation rate from the pool is calculated by the formulas in the Yellow Book as well as with ARGOS and HPAC as described in chapter 3.1. The resulting times before all liquid ammonia has evaporated is given in Table 5.3.

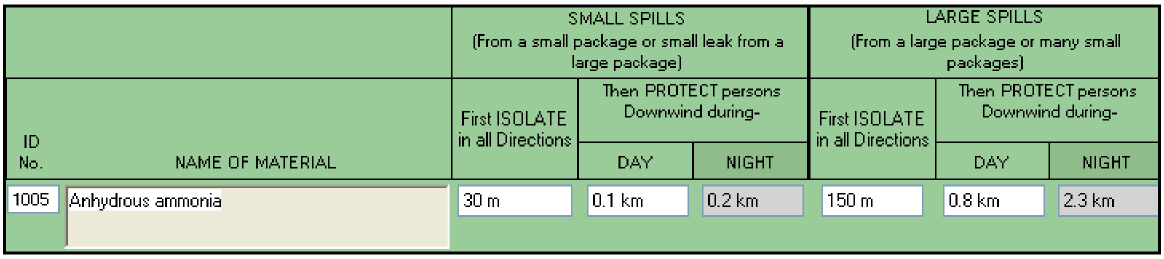
		Time before all ammonia has evaporated (min)		
Vignette	Temperature (°C)	Yellow Book 1)	ARGOS 2)	HPAC
Kjeller 1	-15	280	120	230
Kjeller 2	14	40	86	18
Kjeller 3	6	55	98	11

Table 5.3 Time before all liquid ammonia has evaporated during the releases at Kjeller.
1) No material parameters for asphalt are given in the Yellow Book. In these calculations, the parameters from ARGOS have been used
2) time taken from source module output

5.2 Hazard prediction and assessment tools

5.2.1 Emergency Response Guidebook

The printout from CANUTEC ERG2008 is given in Figure 5.1 below [5]. The distances in ERG2008 are given for small spills (less than 200 litres for liquids and 300 kg for solids) and for large spills (greater than 200 litres for liquids and 300 kg for solids) separately. Different isolation zones and PADs are given for day-time and night-time releases.



		SMALL SPILLS (From a small package or small leak from a large package)			LARGE SPILLS (From a large package or many small packages)		
		First ISOLATE in all Directions	Then PROTECT persons Downwind during-		First ISOLATE in all Directions	Then PROTECT persons Downwind during-	
ID No.	NAME OF MATERIAL		DAY	NIGHT		DAY	NIGHT
1005	Anhydrous ammonia	30 m	0.1 km	0.2 km	150 m	0.8 km	2.3 km

Figure 5.1 Printout of ammonia release from ERG2008.

The ammonia release discussed in the current report is defined as a large spill occurring during day-time. According to ERG2008, one should then first isolate **150 m** in all directions around a large spill and then protect persons **0.8 km** downwind.

5.2.2 ”Farlig gods”

The method for calculation of safety distances in ”Farlig gods” is simple, and temperature is the only required input parameter [6]. The program calculates the vapour pressure at the given temperature, and it is assumed that the vapour pressure in kPa corresponds directly to a

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[14] Surface roughness of asphalt is not defined in TNO Yellow Book

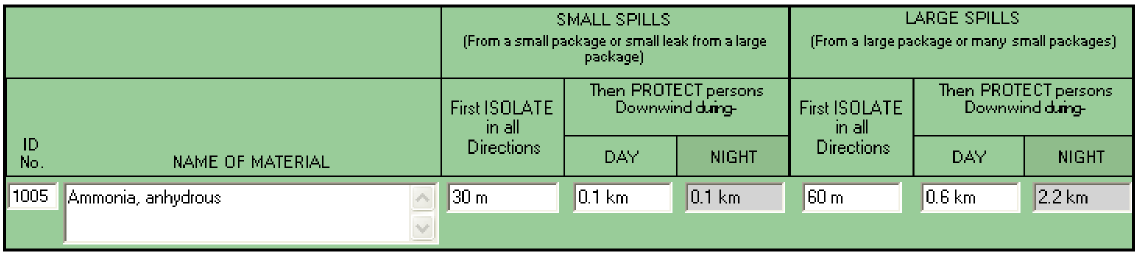
recommended safety distance (1 kPa = 1m) (Table 5.4). It should be noted that DSB recommends that this function is applied with caution, and that the method should be limited to toxic gases and large accidents (tanker trucks and rail wagons). The safety distances are guidelines only and intended for the acute phase.

	Temperature		
	Winter (-15°C)	Summer (14°C)	Autumn (6 °C)
Safety distance (m)	232	715	537

Table 5.4 Ammonia safety distances given by DSB "Farlig gods".

5.3 NBC-Analysis

NBC-Analysis calculates attack areas and hazard areas as described in Chapter 2.3. For toxic industrial chemicals, NBC-Analysis uses the data from ERG2004 shown in Figure 5.2. Note that these isolation distances and protection action distances are different from the current 2008 version of ERGO (see Chapter 2.2.1).



		SMALL SPILLS (From a small package or small leak from a large package)			LARGE SPILLS (From a large package or many small packages)		
		First ISOLATE in all Directions	Then PROTECT persons Downwind during-		First ISOLATE in all Directions	Then PROTECT persons Downwind during-	
ID No.	NAME OF MATERIAL		DAY	NIGHT		DAY	NIGHT
1005	Ammonia, anhydrous	30 m	0.1 km	0.1 km	60 m	0.6 km	2.2 km

Figure 5.2 Printout of ammonia release from ERG2004.

NBC-Analysis produces a circular "release area", which is the predicted area immediately affected by the release (equals the initial isolation zone from ERGO). In the current scenario (a large release), a circular release area with radius 60 m is predicted [7].

Secondly, NBC-Analysis produces a "hazard area", in which unprotected personnel may be affected by the agent spreading downwind from the "release area". In case of an extra large spill (defined as greater than 1500 kg), the protective action distance given in ERGO should, according to NBC-Analysis, be doubled. The shape of the hazard area obtained by NBC-Analysis is dependant of the wind speed: If the wind speed is below or equal to 10 km/h (2.78 m/s), a circular hazard area is produced; if the wind speed is above 10 km/h, a hazard area with a triangular shape is produced.

In vignette 1 (winter) the wind speed is 7.2 km/h (2 m/s) and a circular hazard area with radius 1.2 km is therefore produced at daytime[15] (Figure 5.3). In vignette 2 and vignette 3 (summer and autumn), the wind speed is above 10 km/h, and a triangular hazard area, which extends 1.2 km downwind from release is produced (Figure 5.4). The area affected is 30 degrees on each side of the centreline.

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[15] NBC-Analysis defines the time 0600Z as day-time. If the release had taken place during night-time, the radius or the downwind distance of the hazard area would have been 4.4 km.

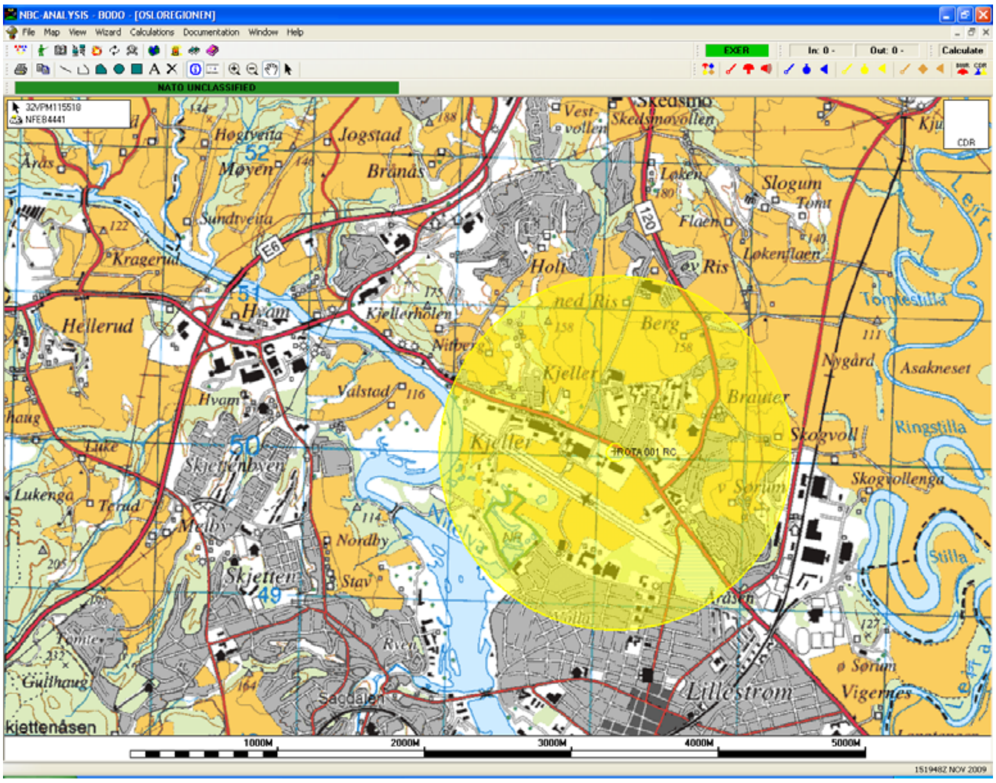


Figure 5.3 Ammonia hazard areas produced by NBC-Analysis after day-time release of ammonia during winter (wind speed below 10 km/h).

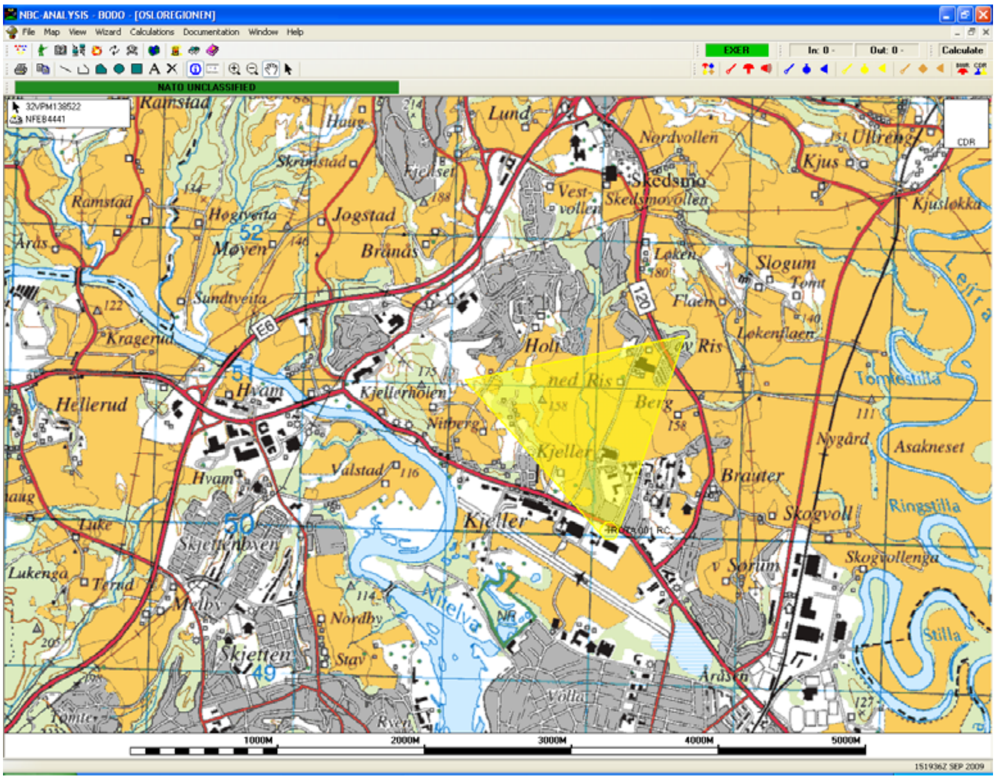


Figure 5.4 Ammonia hazard areas produced by NBC-Analysis after day-time release of ammonia during summer or autumn (wind speed above 10 km/h).

5.4 Dispersion modelling and simulation

For the simulations in HPAC, the surface roughness was taken from the map data. ARGOS uses the surface roughness close to the meteorological tower (entered manually) to set up a wind profile and uses the surface roughness from the map data for the rest of the calculations (see Chapter 2.5.2).

It proved to be difficult to obtain results with DEGADIS for the ammonia scenarios. It was not possible to get results for all three vignettes using the same parameters as for the HPAC and ARGOS simulations. Since DEGADIS is designed for the dispersion of dense gas/aerosol clouds, it is not necessarily optimal to use it for ammonia. Even though pure ammonia is lighter than air, the mixture of ammonia gas and air will initially be denser than the surrounding air. This is because of the heat taken from the air in order to evaporate ammonia aerosols causes the temperature of air to decrease, and this leads to a mixture of air and ammonia that is denser than the surrounding air. Thus, initially ammonia can behave like a dense gas. (This is probably why the possibility to use DEGADIS to calculate the dispersion of ammonia is an option.) However, as the ammonia is dispersed further from the source, the mixture is diluted with pure air, and the density of the mixture will decrease resulting eventually in a light gas. Because of this, no DEGADIS results are included in this section.

Vignette 1: Constructed meteorological conditions at winter time

Height (m)	Pressure (Pa)	Temp (°C)	Wind **from** (degrees)	Wind speed (km/h) [1)]	Stability	RH (%)	Cloud cover
Ground level	101325	-15	167	7.2 (2.0 m/s)	Moderately stable (F)	70-79	Clear sky

Table 5.5 Meteorological conditions from Kjeller at 0600Z (constructed).
[1)] at 10 m height

The meteorological data for this vignette are given in Table 5.5. In this vignette, it was planned to incorporate an inversion at 200 m height. However, when using the manual weather input, ARGOS has no possibility to specify that there is an inversion layer. This could be specified if meteorological data imported from meteorological services are used (called numerical weather prediction data, NWP, in ARGOS), but this has not been used in the current simulations.

When using manual weather input in ARGOS, the prediction can be improved by using weather data from more than one height (as used in one of the vignettes at Ørland). In the current simulations however, only weather data from one height has been used.

Figure 5.5 shows the maximum areas affected by the different concentration levels in the horizontal plane as calculated with ARGOS (as black lines) and HPAC. Figure 5.6 shows the vertical areas affected calculated with HPAC. Table 5.6 gives the maximum downwind distances, widths and heights of the plume.

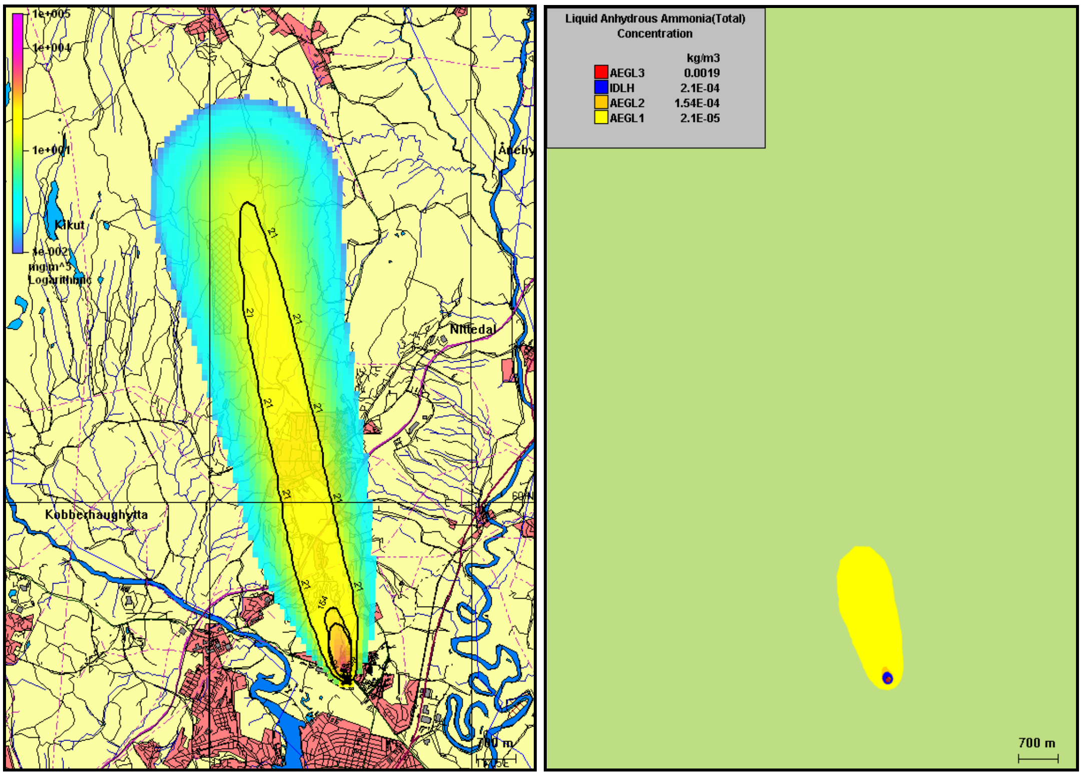


Figure 5.5 *Release of 10 000 kg ammonia at Kjeller (1 200 kg as gas and aerosols and 8 800 kg as liquid) modelled by ARGOS at left and by HPAC at right (using the same scale). The liquid evaporates during 127 min in ARGOS and 230 min in HPAC. The temperature is -15 °C and the wind speed is 2 m/s from 167°. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3). The areas obtained by ARGOS are given as black lines.*

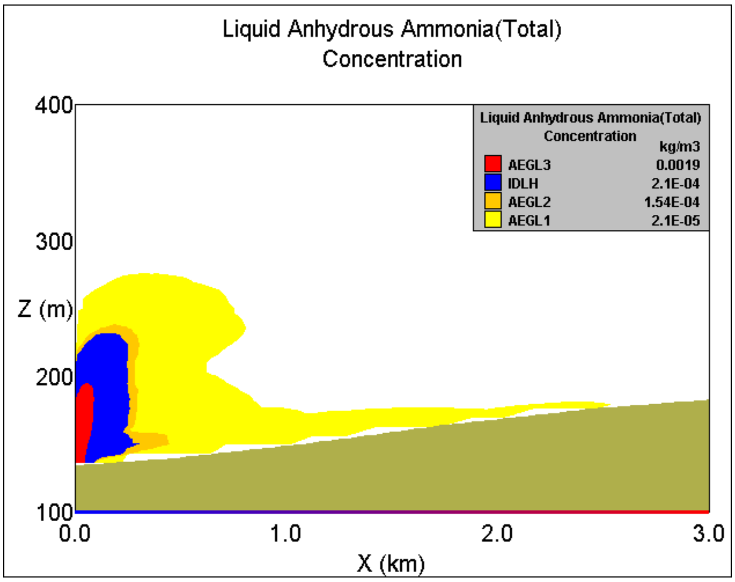


Figure 5.6 *Release of 10 000 kg ammonia at Kjeller (1 200 kg as gas and aerosols and 8 800 kg as liquid) modelled by HPAC. The liquid evaporates during 230 min. The temperature is -15 °C and the wind speed is 2 m/s from 167°. The plot shows the maximum vertical downwind areas affected by the different concentrations (AEGL-1, AEGL-2, IDLH and AEGL-3). The green area represents the ground.*

Software	Concentration limit	Max distance (km)	Max width (km)	Max height of plume (m)
HPAC	AEGL-1	2.3 (32 min)	0.90 (27 min)	130 (240 s)
	AEGL-2	0.24 (81 min)	0.18 (27 min)	100 (155 s)
	IDLH	0.16 (77 min)	0.17 (28 min)	95 (145 s)
	AEGL-3	0.05 (15 s)	0.09 (15 s)	60 (80 s)
ARGOS	AEGL-1	8.6 (60 min)	0.90 (21 min)	NA
	AEGL-2	1.4 (15 min)	0.38 (10 min)	NA
	IDLH	1.0 (12 min)	0.35 (9 min)	NA
	AEGL-3	0.19 (4 min)	0.10 (2 min)	NA

Table 5.6 *Maximum distance the ammonia cloud travels, maximum width of the cloud and maximum height of the plume above ground after a release during winter time. NA: Not applicable*

In Figure 5.7, the evaporation rates from Yellow Book, ARGOS and HPAC are compared. ARGOS has the highest evaporation rate and Yellow Book the lowest rate, with HPAC in the middle.

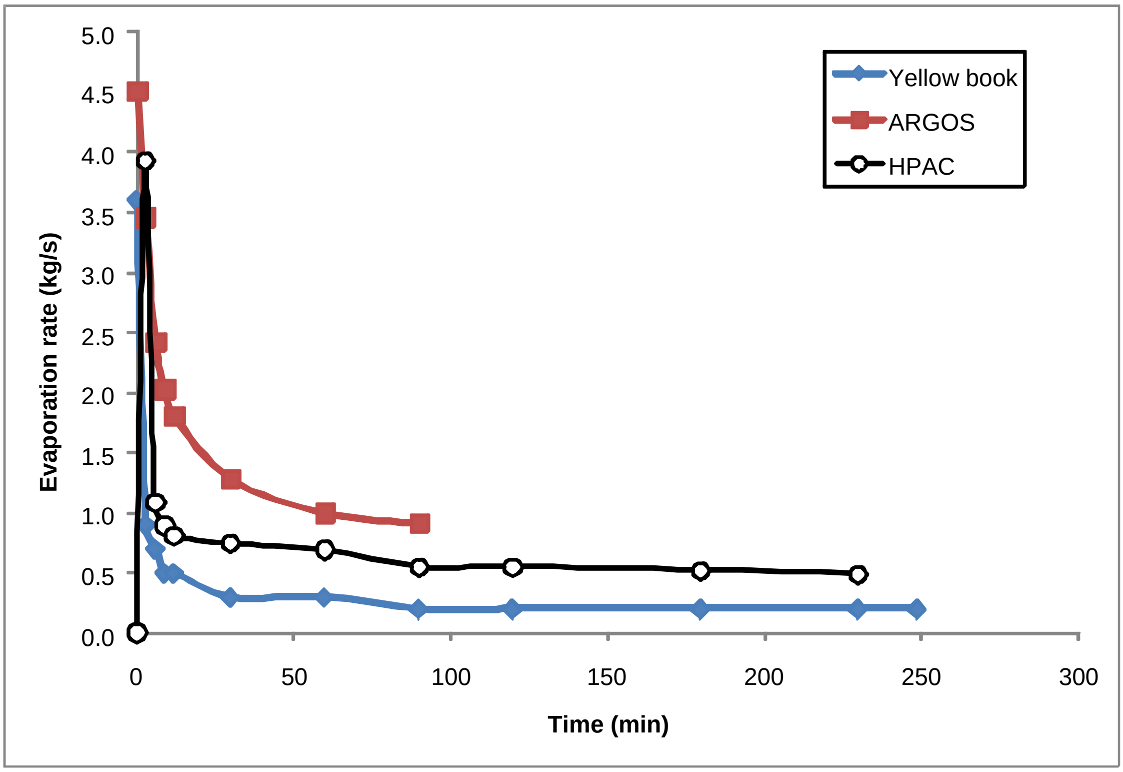


Figure 5.7 *Comparison of ammonia evaporation rates on asphalt calculated using the Yellow Book method, the ARGOS source term module, and HPAC.*

Vignette 2: Summer

Height (m)	Pressure (Pa)	Temp (°C)	Wind from (degrees)	Wind speed (km/h) [1)]	Stability	RH (%)	Cloud cover
Ground level	101325	14	167	23 (6.4 m/s)	Moderately Unstable (B)	90-100	100% covered

Table 5.7 Meteorological conditions at Kjeller 16 July 2009 at 1200Z.
[1)] at 10 m height

The meteorological parameters for vignette 2 are given in Table 5.7. Figure 5.8 shows the maximum areas affected by the different concentration levels in the horizontal plane as calculated with ARGOS (black line) and HPAC. Figure 5.9 shows the vertical areas affected calculated with HPAC. Table 5.8 gives the maximum downwind distances, the maximum width and maximum height of the plume.

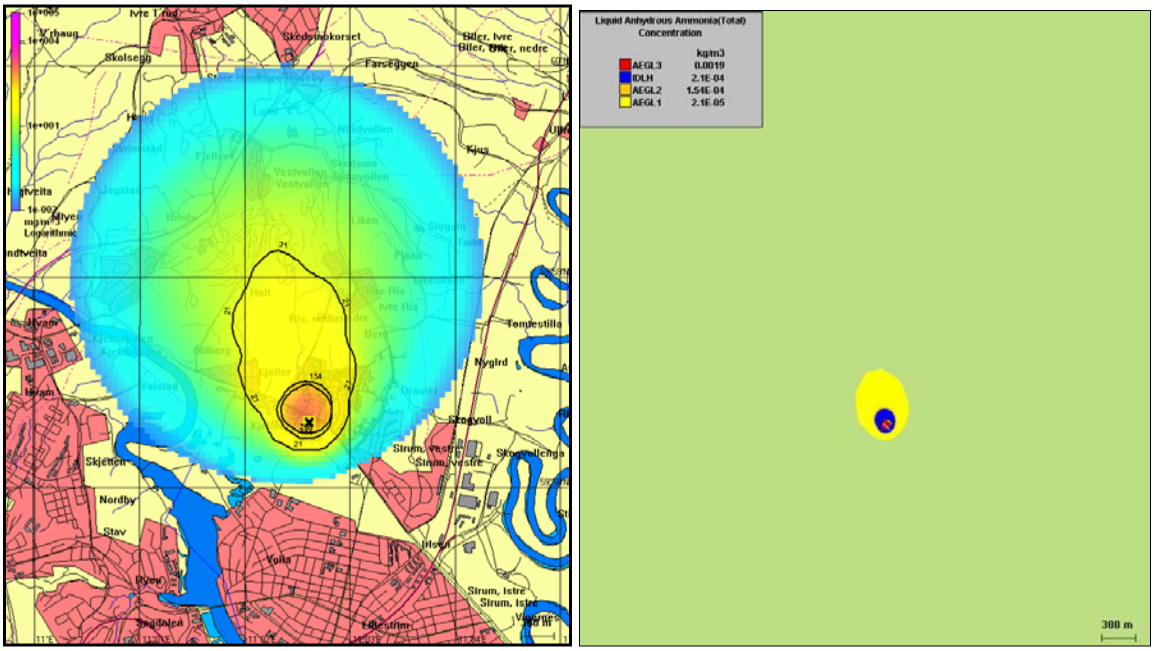


Figure 5.8 Release of 10 000 kg ammonia at Kjeller (3 000 kg as gas and aerosols and 7 000 kg as liquid) modelled by ARGOS at left and by HPAC at right (using the same scale). The liquid evaporates during 24 min in ARGOS and 18 min in HPAC. The temperature is 14 °C and the wind speed is 6.4 m/s from 167°. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3). AEGL-3 concentration is never reached in ARGOS. The areas obtained by ARGOS are given as black lines.

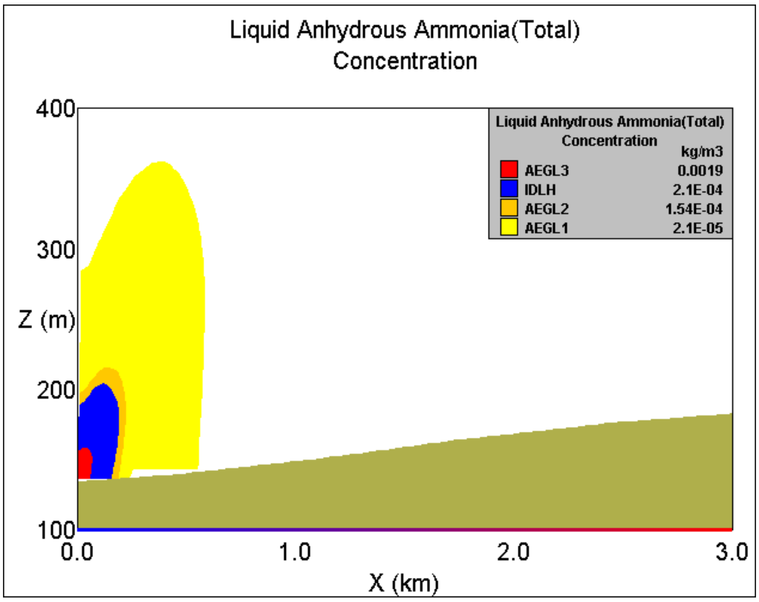


Figure 5.9 Release of 10 000 kg ammonia at Kjeller (3 000 kg as gas and aerosols and 7 000 kg as liquid) modelled by HPAC. The liquid evaporates during 18 min. The temperature is 14 °C and the wind speed is 6.4 m/s from 167°. The plot shows the maximum vertical downwind areas affected by the different concentrations (AEGL-1, AEGL-2, IDLH and AEGL-3). The green area represents the ground.

Software	Concentration limit	Max distance (km)	Max width (km)	Max height of plume (m)
HPAC	AEGL-1	0.51 (80 s)	0.46 (60 s)	220 (85 s)
	AEGL-2	0.17 (25 s)	0.21 (20 s)	80 (35 s)
	IDLH	0.15 (20 s)	0.18 (20 s)	70 (25 s)
	AEGL-3	0.05 (15 s)	0.08 (10 s)	20 (10 s)
ARGOS	AEGL-1	1.6 (4 min)	1.0 (2 min)	NA
	AEGL-2	0.36 (1 min)	0.49 (1 min)	NA
	IDLH	0.34 (1 min)	0.44 (1 min)	NA
	AEGL-3	Not reached	Not reached	NA

Table 5.8 Maximum distance the ammonia cloud travels, maximum width of the cloud and maximum height of the plume above ground after a release during summer time. NA: Not applicable

The minimum time step in ARGOS is 1 min. After the first time step, 1 minute, the concentration in the plume is at the IDLH level. The cloud does not reach AEGL-3 level in this scenario using ARGOS. HPAC predicts a concentration at the AEGL-3 level after 10 s.

Vignette 3: Autumn

Height (m)	Pressure (Pa)	Temp (°C)	Wind from (degrees)	Wind speed (km/h) [1)]	Stability	RH (%)	Cloud cover
Ground level	101325	6	167	32 (8.9 m/s)	Very Unstable (A)	70-79	>50 % covered

Table 5.9 Meteorological conditions from Kjeller 29 Oct 2009 at 1200Z.
1) at 10 m height

The meteorological parameters for vignette 3 are given in Table 5.9. Figure 5.10 shows the maximum areas affected by the different concentration levels in the horizontal plane as calculated with ARGOS (as black lines) and HPAC. Figure 5.11 shows the vertical areas affected calculated with HPAC. Table 5.10 gives the maximum downwind distances, the maximum width and maximum height of the plume.

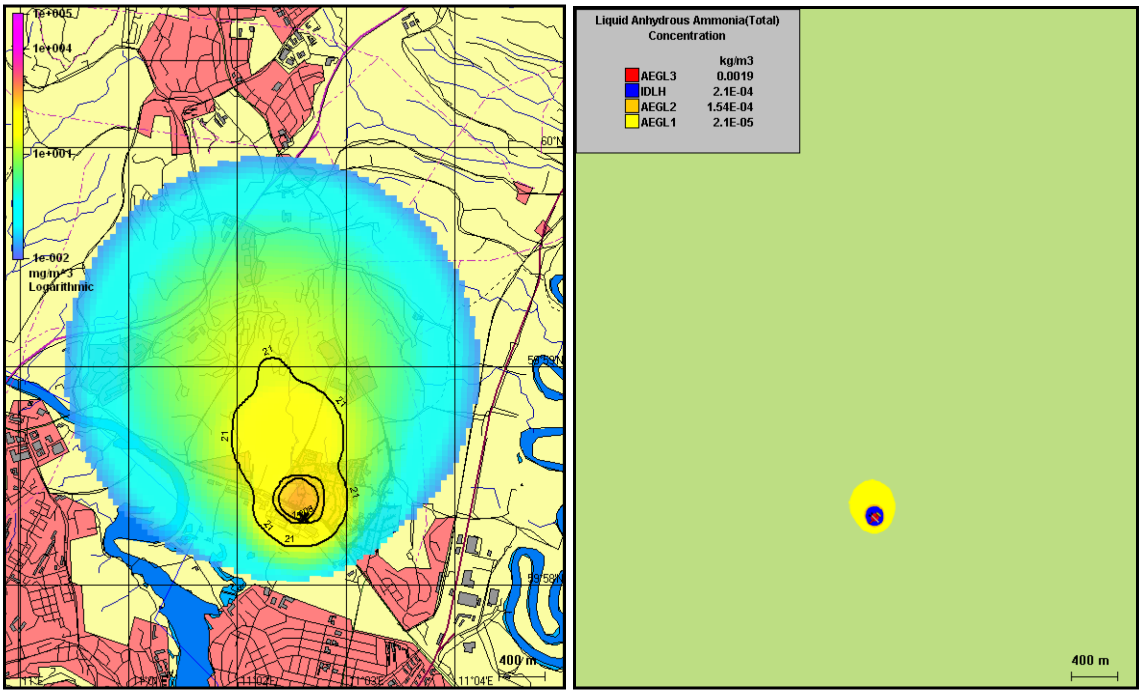


Figure 5.10 Release of 10 000 kg ammonia at Kjeller (2 400 kg as gas and aerosols and 7 600 kg as liquid) modelled by ARGOS at left and by HPAC at right (using the same scale). The liquid evaporates during 5 min in ARGOS and 11 min in HPAC. The temperature is 6 °C and the wind speed is 8.9 m/s from 167°. The plots show the total areas affected by the specified concentration levels (AEGL-1, AEGL-2, IDLH and AEGL-3). AEGL-3 concentration is never reached in ARGOS. The areas obtained in ARGOS are given as black lines.

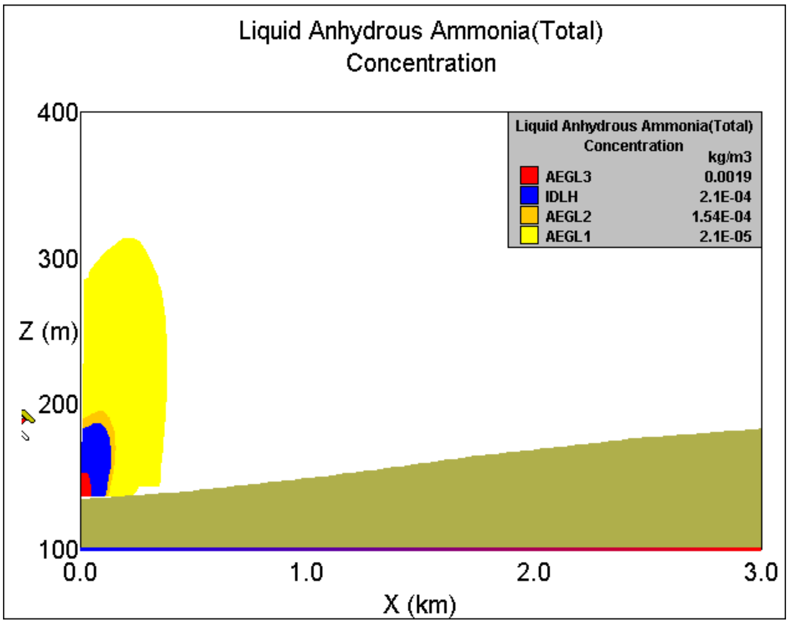


Figure 5.11 Release of 10 000 kg ammonia at Kjeller (2 400 kg as gas and aerosols and 7 600 kg as liquid) modelled by HPAC. The liquid evaporates during 11 min. The temperature is 6 °C and the wind speed is 8.9 m/s from 167°. The plot shows the maximum vertical downwind areas affected by the different concentrations (AEGL-1, AEGL-2, IDLH and AEGL-3). The green area represents the ground.

Software	Concentration limit	Max distance (km)	Max width (km)	Max height of plume (m)
HPAC	AEGL-1	0.33 (35 s)	0.39 (30 s)	175 (25 s)
	AEGL-2	0.12 (10 s)	0.17 (5 s)	60 (15 s)
	IDLH	0.10 (10 s)	0.15 (5 s)	50 (15 s)
	AEGL-3	0.04 (5 s)	0.06 (5 s)	15 (5 s)
ARGOS	AEGL-1	1.4 (3 min)	0.95 (2 min)	NA
	AEGL-2	0.37 (1 min)	0.44 (1 min)	NA
	IDLH	0.33 (1 min)	0.34 (1 min)	NA
	AEGL-3	Not reached	Not reached	NA

Table 5.10 Maximum distance the ammonia cloud travels, maximum width of the cloud and maximum height of the plume above ground after a release during autumn.
NA: Not applicable

The minimum time step in ARGOS is 1 min. After the first time step, 1 minute, the concentration in the plume is at the IDLH level. The cloud does not reach AEGL-3 level in this scenario using ARGOS. HPAC predicts a concentration at the AEGL-3 level after 5 s.

5.5 Discussion

In this scenario, it was planned to include a moderate rainfall (2.5-7.6 mm/hr) during the release. However, wash-out effects from rainfall has not yet been implemented in the chemical part of ARGOS [27], but is an important parameter in the modellation after a radiological release. It is also questionable how much effect rainfall will have on the distribution of ammonia [28;29], but this will not be discussed in this report. Ammonia is soluble in water, and it is not unlikely that rainfall therefore could have an effect. Ammonia (NH_3) will react with atmospheric water to produce an HNO_3 mist, which behaves differently than ambient temperature NH_3 [4]. It is possible to define rainfall and also inversion layers in NBC-Analysis. This does not, however, affect the results from the release of industrial chemicals, because these results are taken from the emergency response guidebook (ERG2004) [30].

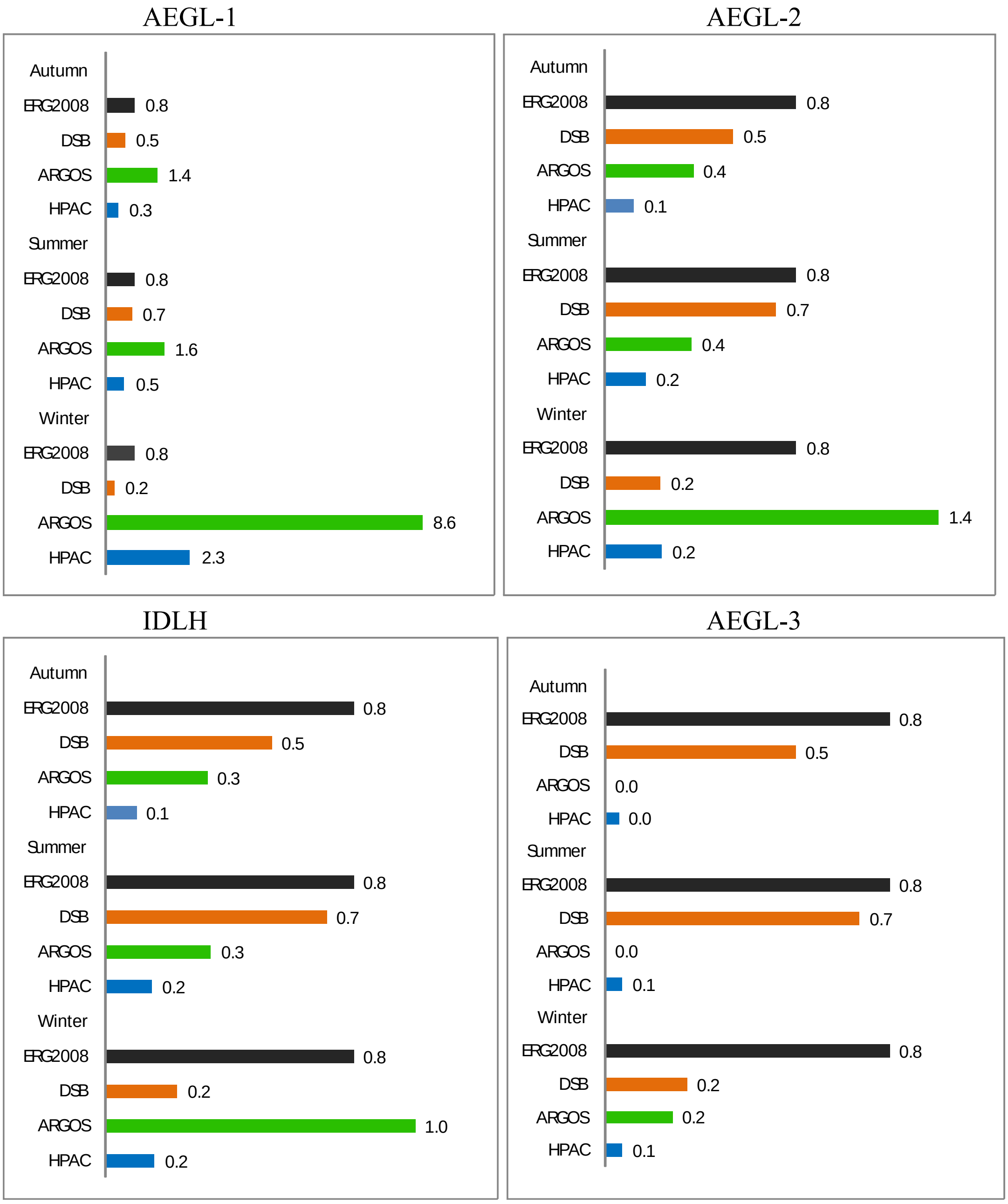


Figure 5.12 Maximum distance (in km) the ammonia cloud travel before the concentration drops below the concentration limits AEGL-1 (top left), AEGL-2 (top right), IDLH (bottom left) and AEGL-3 (bottom right) for the three times of year tested. The protection action distance from ERGO and the safety distance from DSB "Farlig gods" is included.

ERGO discriminates between releases at day-time or night-time. In the scenarios presented here, all releases have taken place during day-time.

From Figure 5.5, Figure 5.8, Figure 5.10 and Figure 5.12, it can be seen that the distance the plume is dispersed downwind is generally much larger as simulated by ARGOS than by HPAC. This is in contrast to the results from chlorine release at Ørland MAS, where the hazard distances obtained by ARGOS and HPAC were more similar. HPAC includes dynamic buoyant effects due to lighter-than-air materials, while ARGOS does not include such effects. A lighter-than-air substance will rise faster than neutral materials with density comparable to air or dense gases. HPAC may therefore predict that the ammonia plume will rise above the ground while ARGOS may predict that the plume will persist at ground level for a longer time. Since the horizontal areas in the figures are taken at surface level, this could explain why the distance downwind is smaller with HPAC than with ARGOS. From Figure 4.7, Figure 4.18, Figure 4.20, Figure 5.6, Figure 5.9 and Figure 5.11 it is evident from HPAC that the ratio of the height of the plume to the downwind distance is much larger for the ammonia scenario than for the chlorine scenario.

Figure 5.12 shows that the ammonia cloud travels much longer during winter time in low temperature, low wind and stable atmosphere than during autumn and summer with higher temperature, more unstable atmosphere and higher wind speed. It is thought that the wind speed and atmospheric stability have the greatest effect on the dispersion of the vapour cloud, whereas the temperature will mainly affect the mass of the initial cloud (gas and aerosols as seen in Table 5.2).

The highest concentration level (AEGL-3) under autumn and summer conditions was never reached by ARGOS. This is probably due to the fact that the minimum time step in ARGOS is one minute. The concentrations above AEGL-3 obtained by HPAC have disappeared before one minute has passed.

The maximum height of the plume calculated by HPAC is largest during summer at moderately unstable atmosphere (vignette 2) and smallest during winter at moderately stable atmosphere (vignette 1). During autumn conditions with very unstable atmosphere (vignette 3), the maximum height is between the other two simulations. One could perhaps expect that the vertical distribution would be largest the more unstable the atmosphere is. However, vignette 3, which have the most unstable atmosphere, also have the largest wind speed. In addition, because of the temperature, the initial cloud is larger in vignette 2 than vignette 3. Also, the more unstable the atmosphere is, the more turbulent mixing is present in the vertical direction and consequently more air is mixed into the plume. This will create a more dilute plume than with a more stable atmosphere, and thus high concentrations may not reach as high.

The areas affected by the ammonia cloud, as predicted by NBC-Analysis and ERG2008, are in the ranges obtained by HPAC and ARGOS for the AEGL-1 concentration level (i.e. non disabling concentration). The safety distance predicted by DSB ”Farlig gods” is in the AEGL-1 range during summer and autumn conditions and in the IDLH/AEGL-3 range during winter conditions.

The ”Farlig gods” program predicts larger safety areas during summer conditions compared to winter conditions. This is in contradiction to the results from HPAC and ARGOS, and occurs because the safety distance given by the ”Farlig gods” program depends only on the vapour pressure, which is dependent on the temperature but not wind speed or atmospheric stability. The vapour pressure is much smaller at a winter temperature of -15 °C than at summer or autumn temperature, and thus the ”Farlig gods” program predicts a smaller safety zone, even though other meteorological parameters may lead to a larger hazard area.

6 Modelling and simulation results for soman release

6.1 Scenario description

In this scenario it is assumed that Bodø MAS is attacked with the nerve agent soman by enemy aircrafts. It was of interest to investigate the applicability of the software packages for a chemical warfare agent attack scenario like this.

Two different vignettes, each with 3 fighter bombers, were constructed:

Vignette 1:	3 bombers, each carrying 16 pieces of 250 kg bombs with 47 kg soman (non-thickened). Total of 48 bombs containing 2256 kg soman
Vignette 2:	3 bombers, each carrying 40 pieces of 100 kg bombs with 34 kg soman (non-thickened). Total of 120 bombs containing 4080 kg soman

The three aircrafts are coming in parallel to the runway, one targeting the military side of the airfield (south side), one targeting the runway itself, and one targeting the civilian side (north side). The input parameters are given in Table 6.1.

The toxicological threshold limits used in these calculations are the median toxicity estimates provided for lethality (lethal concentration (C) multiplied by time (t) for 50 percent population effect (LCt_{50})), incapacitating (severe) effects (ICt_{50}) and threshold (mild) effects (ECt_{50}) [31] given in Table 6.1.

These toxicological threshold estimates apply to 2 min dosages. The ECt_{50} value is so low that concentrations above this limit are predicted for very long distances from the release location. The distances fall outside the limitations of use of these dispersion models for constant wind field approximations. More accurate meteorological input would need to be taken into account. Consequently, this limit is not shown in the resulting plots.

Parameter	Value
Time of day	2200Z
Position (MGRS)	33WVQ 72496186
Compound released	Soman
Total bomb load	2256 kg (vignette 1) 4080 kg (vignette 2)
Toxicological limits [31]	
LCt_{50}	35 mg.min/m^3 = 2100 mg.s/m^3 = 0.0021 kg.s/m^3
ICt_{50} (inhal, vap, severe effects)	25 mg.min/m^3 = 1500 mg s/m^3 = 0.0015 kg.s/m^3
ECt_{50} (inhal, vap, mild effects)	0.4 mg.min/m^3 = 24 mg.s/m^3 = 0.000024 kg.s/m^3

Table 6.1 Input parameters.

The meteorological conditions used in the simulations are shown in Table 6.2 below.

Height (m)	Pressure (Pa)	Temp (°C)	Wind from (degrees)	Wind speed (km/h) 1)	Stability	RH (%)	Cloud cover
Ground level	101325	7	233	12 (3.3 m/s)	Neutral (D)	60-69	<50 % covered

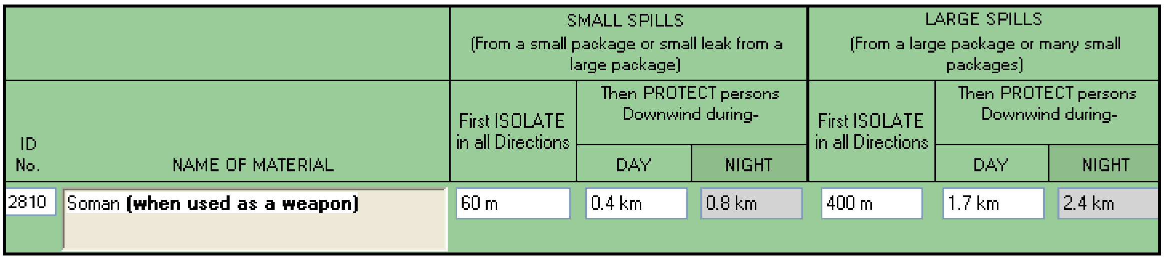
Table 6.2 Meteorological conditions from Bodø 17July 2009 at 2200Z.
1) at 10 m height

The surface roughness of the meteorological tower (see Chapter 2.5.2) is set to rangeland (0.1 m).

6.2 Hazard prediction and assessment tools

6.2.1 Emergency Response Guidebook

The printout from CANUTEC ERG2008 is given in Figure 6.1 below. The distances in ERG2008 are given for small spills (less than 200 litres for liquids and less than 300 kg for solids) and for large spills (greater than 200 litres for liquids and greater than 300 kg for solids) separately [5]. Different isolation zones and PADs are given for day-time and night-time releases.



		SMALL SPILLS (From a small package or small leak from a large package)			LARGE SPILLS (From a large package or many small packages)		
		First ISOLATE in all Directions	Then PROTECT persons Downwind during-		First ISOLATE in all Directions	Then PROTECT persons Downwind during-	
ID No.	NAME OF MATERIAL		DAY	NIGHT		DAY	NIGHT
2810	Soman **(when used as a weapon)**	60 m	0.4 km	0.8 km	400 m	1.7 km	2.4 km

Figure 6.1 Printout of a soman release from ERG2008.

The release of the nerve agent soman discussed in the current report is defined as a large spill occurring during night-time. According to ERG2008, one should first isolate **400 m** in all directions around a large spill of soman and then protect persons **2.4 km** downwind during night-time. It should, however, be noted that ERGO is not designed to handle such cold-war attacks and will therefore probably underestimate the hazard.

6.2.2 ”Farlig gods”

The safety distance is not defined for soman in the ”Farlig gods perm” from DSB [6].

6.3 NBC-Analysis

The current version of NBC-Analysis, based on NATO ATP-45(C) [7], is in particular constructed to deal with ”Cold-war” scenarios like this.

NBC-Analysis calculates attack areas and hazard areas as described in Chapter 2.3. Since the delivery means is air bombs, according to ATP-45(C) (paragraph 1207, p 12-3) the attack area is a circle with radius 2 km. In ATP-45 (C) [7], the area of the attack area is larger for attacks with bombs, air burst rockets, missiles and for unknowns, than for other delivery means.

According to ATP-45(C), soman is a persistent agent which means that downwind distance of the hazard area will never be larger than 10 km (ATP-45(C) paragraph 1212, p 12-11). With a wind speed larger than 10 km/h, the hazard area is defined as a 60° sector with the times before arrival of the soman plume given in Table 6.3 below. The uncertainties in the available information of the weapon load in operational situations are assumed to be large. The two different combinations of bomb loads will therefore, by design, not give any difference in the output from NBC-Analysis, and the results from vignette 1 and vignette 2 are equal. Two plots from NBC-Analysis used on vignette 2 are shown in Figure 6.2. Precipitation during the release did not alter the results.

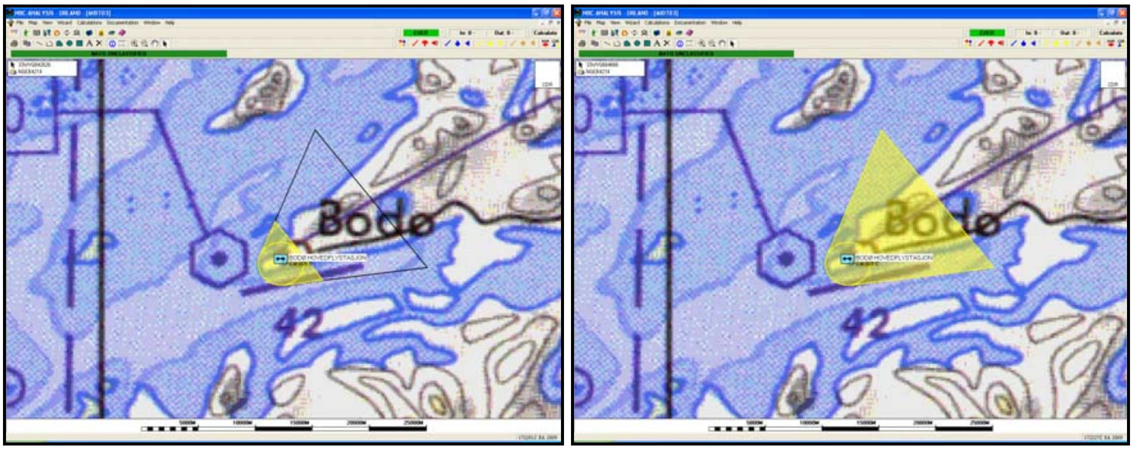


Figure 6.2 Plot from NBC-Analysis after the attack on Bodø MAS with three aircrafts, each dropping 40 bombs containing 34 kg soman (vignette 2). Yellow shaded area is the "attack area" (small circle) and "hazard area" (triangle) according to ATP-45 (C) after 1 min (left) and after 27 min (right).

Time (min)	Distance (km)
1	2.2
2	2.5
5	3.5
10	5.0
15	6.5
20	8.0
25	9.5
27	10

Table 6.3: Time before arrival of the soman plume (the two vignettes give equal results).

The predicted attack and hazard areas are calculated directly after an attack has occurred and is reported as an NBC-3 message. After a survey by use of detection materiel has been conducted and the areas of actual contamination have been defined, these areas should be recalculated and reported by use of NBC-5 and NBC-6 messages.

If a non-persistent agent (e.g. sarin) had been used, the hazard area had been much larger (not shown in this report). With the meteorological conditions described above, the maximum hazard area for sarin would be 30 km. It is also possible to define the time which a volatile agent (like sarin) will persist in the area (duration). NBC-Analysis can then also calculate the time before the hazard disappears. The results from these calculations should be treated with caution, because they are very dependant on the meteorological conditions and on the properties of the surface.

6.4 Dispersion modelling and simulation

The standard values for the air attack suggested by HPAC (shown in Table 6.4) have been used in these simulations. These standard values could be changed, if needed.

	Vignette 1 (large bombs)	Vignette 2 (small bombs)
Mass of load for each munition[16]	47 kg	34 kg
Total mass of agent	2256 kg	4080 kg
Height of burst	15.0 m	15.0 m
Initial size[17]	10.0 m	8.0 m
Median mass diameter (MMD)[18]	500.0 µm	500.0 µm
Sigma D[18]	2.0	2.0
Agent purity	100.0 %	100.0 %
Vapour fraction[19]	15.0 %	15.0 %
Liquid fraction[19]	65.0 %	65.0 %
Released mass for each munition	37.6 kg	27.2 kg
Total mass released	1805 kg	3264 kg
Spread[20]	100.0 m	100.0 m

Table 6.4 HPAC standard values for the air attack with soman.

As could be seen from Table 6.4, the sum of the vapour fraction and the liquid fraction is 80 % (i.e. less than the original mass). The reason for this is that 20 % of the agent is lost during the explosion.

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[16] Agent payload of the munition including impurities. If the agent is not pure, the “Agent purity” factor shold be modified accordingly

[17] Diameter of the initial agent release expressed as a standard deviation

[18] Describes the lognormal size distribution of liquid drops from a release

[19] The sum of the vapour fraction and the liquid fraction may not sum up to 100 % because some agent will be lost during the esplosion

[20] The diameter of the target area over which the munition are distributed

Vignette 1 - 752 kg soman pr aircraft

The maximum downwind distances of the areas affected by dosages corresponding to the limits Mild ECt_{50}, Sev ICt_{50} and LCt_{50} from the air attack with the smallest bombs (vignette 1) are shown in Table 6.5 below.

Dosage limit	HPAC - max distance (km)	ARGOS - max distance (km)
Mild ECt_{50}	>100 1)	>100 1)
Sev ICt_{50}	1.8	24 (105 min)
LCt_{50}	1.4	13 (60 min)

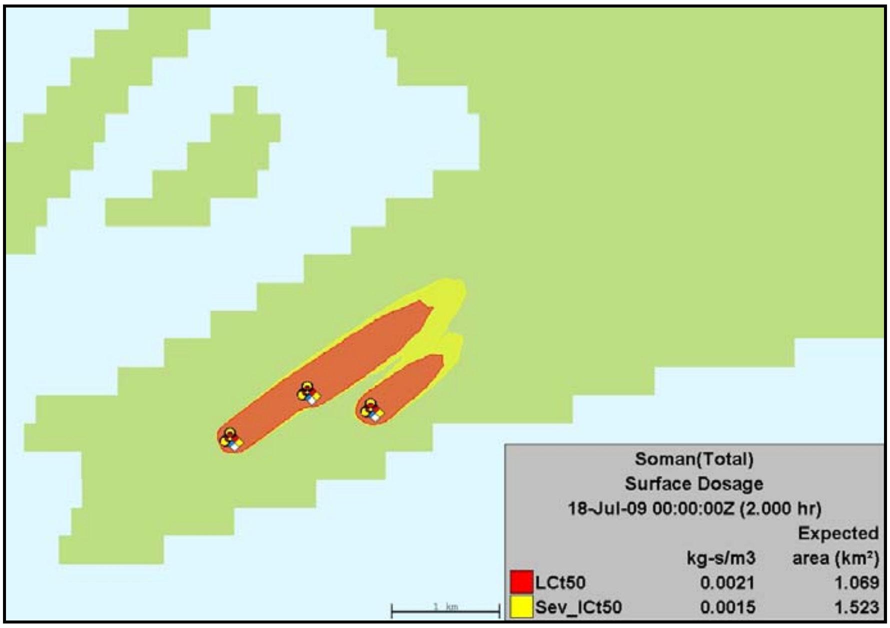
Table 6.5 Maximum travel distances obtained by HPAC and ARGOS for different toxicological limits. The maximum travel distance for Mild ECt_{50} for ARGOS is not presented because the meteorological parameters are not valid for such long distances.
1) The meteorological data is not considered valid above 100 km

ARGOS does not include the possibility to enter air bombs as input. It was therefore decided to release 15% of the bomb loads at a height 15 m above ground and 65 % of the bomb loads directly on the ground. This was considered the most realistic use of the standard input parameters used by HPAC (Table 6.4). The rest (20 %) is in HPAC assumed to be destroyed during the explosion. Thus, for ARGOS in this vignette, 112.8 kg soman was released in the air 15 above ground and 488.8 kg soman was released on the ground for each aircraft (total 1804.8 kg for three aircrafts). The results obtained from ARGOS are shown in Table 6.5.

The maximum distance at the mild ECt_{50} level for ARGOS is not presented because the cloud travels in excess of 100 km and the results are not considered correct since only the meteorological parameters for the release site has been used. ARGOS has implemented a long-distance-puff-distribution-parameterisation which should give reasonable results up to about 1000 km [32]. The model should, however, be used with caution over such long distances because the results will be dependent of weather situations and difficult terrain in the large area of concern, in addition to the type and amount of agent released [33]. The width of the plume is mainly affected by the distance between the dropped bombs and is therefore not included here.

It was also tested to release all the soman at 15 m height above ground and nothing directly on the ground. This simulation showed that differences in release height did not change the results very much.

The dosages in the air close to the ground (surface dosages) obtained by HPAC are shown in Figure 6.3 (left) below. In Figure 6.3 (right), the amount of soman deposited on the ground is shown.



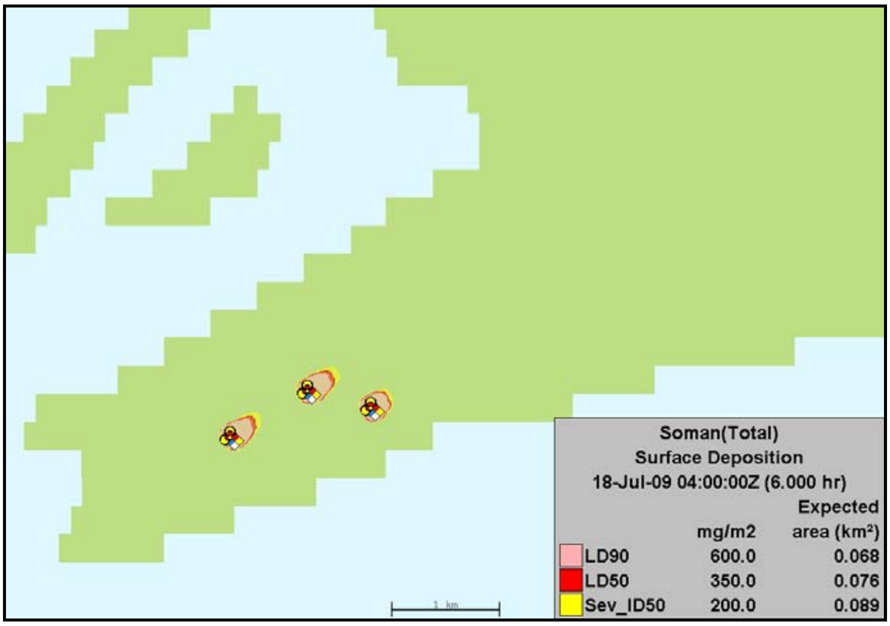


Figure 6.3 Surface dosages from vignette 1 (top) and surface deposition from vignette 1 (bottom), both modelled by HPAC.

A graphical presentation of the dosages obtained at centreline by HPAC and ARGOS at different distances (10, 5, 3 and 1 km) from the release site is shown in Figure 6.4 below. It shows that ARGOS predicts a very steep rise in dosage with time, whereas the rise predicted by HPAC is more gentle.

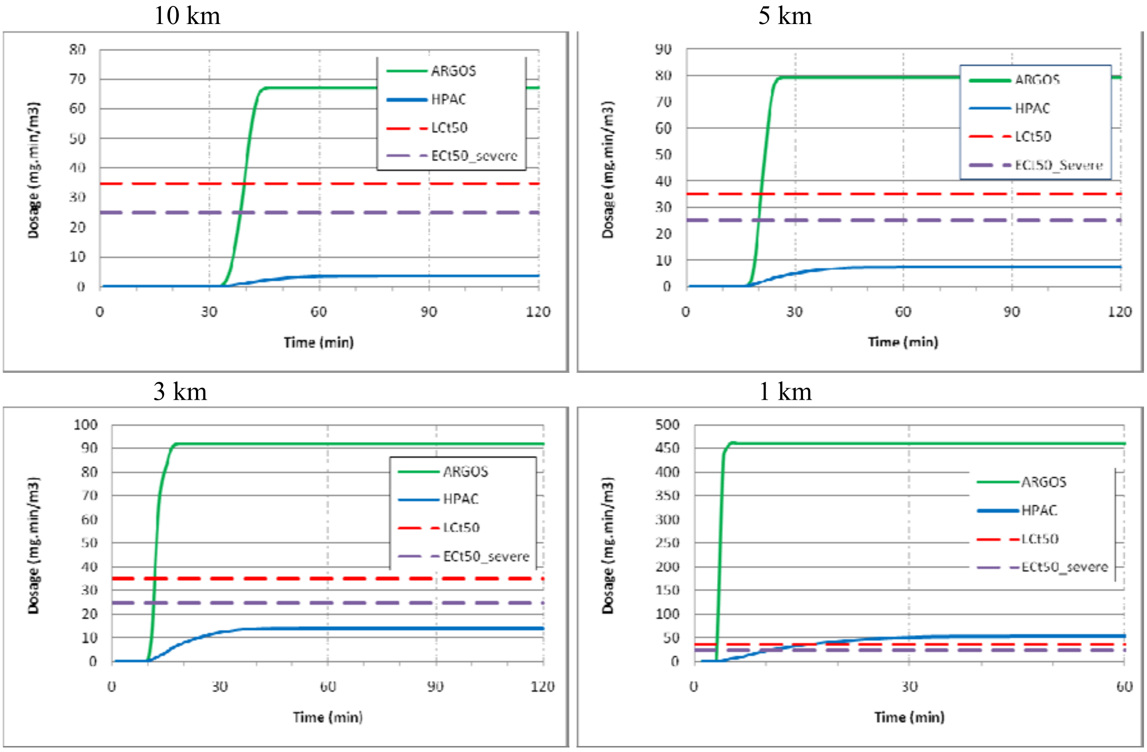


Figure 6.4 Dosages obtained at centreline by HPAC and ARGOS at different distances (10, 5, 3 and 1 km) from the release site.

Vignette 2: 1360 kg soman pr aircraft

The results from the air attack with the largest bombs (vignette 2) are shown in Table 6.6 below. In this vignette, 204 kg soman was released in the air 15 above ground and 884 kg soman was released on the ground for each aircraft (total of 3264 kg for three aircrafts) in the simulations carried out by ARGOS.

Program	Dosage limit	Max distance (km)			
		Surface roughness from map	Urban (roughness 1 m)	Rangeland (roughness 0.1 m)	Barren land (roughness 0.002 m)
HPAC	Mild ECt_{50}	>100 1) NA	NA	NA	NA
	Sev ICt_{50}	3.4 (60 min)	NA	NA	NA
	LCt_{50}	2.2 (60 min)	NA	NA	NA
ARGOS	Mild ECt_{50}	NA	Not presented	Not presented	Not presented
	Sev ICt_{50}	NA	25 (109 min)	31 (122 min)	33 (148 min)
	LCt_{50}	NA	22 (100 min)	26 (106 min)	26 (126 min)

Table 6.6 Maximum travel distances obtained by HPAC and ARGOS at different surface roughness at the meteorological tower. NA: Not applicable
1) The meteorological data is not considered valid above 100 km

In this table, different surfaces close to the meteorological tower have been selected (urban, rangeland, barren land). This surface roughness is in ARGOS used to calculate the wind profile out from the tower. The surface roughness for the rest of the computational domain is taken from the map used.

The width of the plume is mainly affected by the distance between dropped bombs and is therefore not included here (see under vignette 1).

The soman dosages in the air close to the ground (surface dosages) obtained by HPAC are shown in Figure 6.5 (left) below. In Figure 6.5 (right), the amount of soman deposited on the ground is shown.

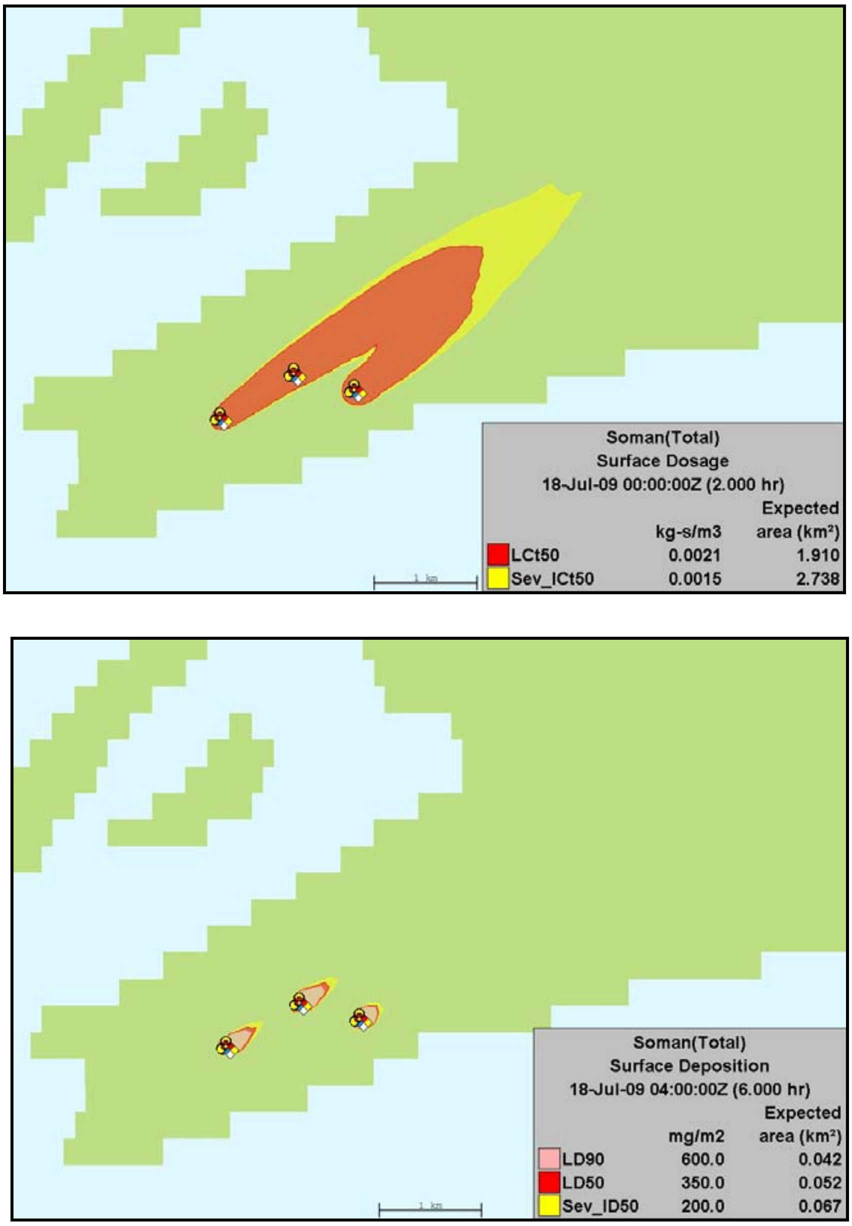


Figure 6.5 Surface dosages from vignette 2 (top) and surface deposition from vignette 2 (bottom), both modelled by HPAC.

6.5 Discussion

In this scenario, the results from HPAC and ARGOS are very different (Table 6.5 and Table 6.6). ARGOS predicts a much larger hazard area compared to HPAC (more than 10 times longer downwind distance). It is not known why HPAC and ARGOS predicts so different hazard areas in this scenario. It is assumed that HPAC is more suitable for a cold war scenario than ARGOS. It is, for example, not possible to specify a bomb load by ARGOS. Soman was with ARGOS therefore released at one point from each aircraft (at two different heights above ground).

The surface roughness close to the meteorological tower has some effect on the output from ARGOS, with barren land giving the largest maximum travel distance and urban the shortest distance.

According to ERG2008, one should first isolate 400 m in all directions around a large spill of soman and then protect persons 2.4 km downwind during night-time. This is quite similar to the LCt_{50} and Sev ICt_{50} distances obtained by HPAC, but is much shorter than the same distances predicted by ARGOS.

NBC-Analysis predicts a hazard area which will never extend more than 10 km downwind. This distance is in agreement with the Severe ICt_{50} level from HPAC, but much shorter than the levels presented by ARGOS. The distances given by NBC-Analysis is meant to be on the safe side and should be lowered when a site survey of the area has been carried out.

7 User experiences

The Emergency Response Guidebook (ERG2008) [5] is a simple guide which gives initial isolation zones and protective action distances very fast. No user input is necessary with this guide, except type of agent. The software is designed to handle transport accidents by road or rail, and discriminates between small spills and large spills and weather the release occurs during night-time or day-time. The protection action distances obtained for the three scenarios presented in this report are in the same range as obtained for AEGL-2 levels for chlorine and AEGL-1 levels for ammonia by using ARGOS and HPAC (except for ARGOS during winter time, were ERGO gives results between AEGL-1 and AEGL-2). For the scenario with soman at Bodø MAS, the results are in the same range as the values from HPAC for severe ICt_{50}. ERGO is, however, not designed to handle "cold war" scenarios like this.

The "Farlig gods" program from DSB [6] is also a very quick guide, which gives more information about the dangerous material than the ERG2008. It gives information about physical and chemical properties of the agent, health-risks associated with the agent and how to deal with fires and environmental releases of the agent. To be able to get safety distances, it is necessary for the user to enter the actual temperature during the release. For the chlorine scenario, this safety distance is much smaller than the distances given by ERG2008 and is in the AEGL-3 range obtained by HPAC and ARGOS (note that the AEGL-3 concentration area calculated with HPAC and ARGOS extend beyond the Farlig gods safety distance). In the ammonia release, the values given by the ”Farlig gods” handbook is in the AEGL-2 range obtained by HPAC and ARGOS. For this scenario, the safety distance is smallest during winter time and largest during summer time, which is opposite to the results obtained by HPAC and ARGOS. The reason for this is that "Farlig gods" calculates a safety distance purely based on the vapour pressure of the substance, which increases with the temperature, but does not take the other meteorological conditions into consideration. The "Farlig gods" handbook does not provide safety distances for the nerve agent soman.

The NBC-Analysis software is a computerised version of NATO ATP-45 (C), and operates in two very different modes when used on an industrial release and on a chemical warfare agent [20]. For industrial compounds it uses an earlier version of the Emergency Response Guidebook (ERG2004), which gives different results compared to the more resent ERG2008[21]. In addition, NBC-Analysis doubles the protective action distances when the release is larger than 1500 kg, which has been the case in the current scenarios. NBC-Analysis, therefore give affected areas in the same range as AEGL-2 for chlorine and AEGL-1 for ammonia. When NBC-Analysis is used on the "cold war" scenario at Bodø MAS, the user needs to enter input parameters about the weather and the weapon used. It is therefore more advanced than ERG2008 and the "Farlig gods" program. It is, however, possible to run the program without knowing all details about the release.

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[21] The coming version av NBC-Analysis (version 12), which will be called CBRN-Analysis, will use the ERGO 2008 version of the ERG Guidelines. This version will be released ultimo 2010.

Especially for a persistent agent like soman, the results will be the same, independent of the selection of weapon parameters. A “chemical attack wizard” is also available in the program, where the only necessary inputs are the location of the attack and some simple meteorological conditions (wind direction, wind speed and atmospheric stability). The weather should preferably be imported automatically from a properly set up meteorological server. The results from NBC-Analysis used at Bodø are between Severe ICt_{50} and Mild ECt_{50} obtained by HPAC, and is similar to the LCt_{50} distance predicted by ARGOS for the small bomb load and about half the LCt_{50} distance predicted by ARGOS for the large bomb load.

HPAC is a program with a very comprehensive code which has undergone much testing and evaluation. Results from these verification experiments are available [34]. It is possible to obtain results with relatively few input data. HPAC then assumes default values for the undefined parameters. The accuracy of the results are, however, much dependent on good input values. The results could differ largely from the true values if for example the meteorological conditions are very different from the default value. HPAC is therefore difficult to use in an operational setting with any kind of confidence. HPAC has a simple user interface, and is used by many NATO-countries. Since HPAC is used within NATO, training courses are available both at the NATO School in Oberammergau, Germany and at DTRA in the USA. It is quite difficult to obtain information about how the calculations are carried out. In addition it has been some problems regarding the release of information about the most recent version of HPAC.

ARGOS is a flexible program which consists of separate modules for handling different release scenarios, both radiological and chemical. The radiological part has been on the market for many years, but the chemical part is relatively new and still under development. ARGOS is a software where all participating countries in the consortium can influence on the content and layout of the program. This could, however, also slow down the development process because all decisions have to be discussed among the participants. A user’s group is available, where all users can participate. The program is quite simple to use and gives rapid answers when the input parameters have been selected. It requires, however, quite a lot of input parameters, which sometimes are difficult to obtain. The results are presented graphically on a map in a nice manner, but with limited possibilities to get numerical outputs. Some information could be obtained by looking into the database entries and XML files generated by the software, but this is for expert users only. The program has, unfortunately, a lot of error messages and non-working options which makes the use a bit confusing, at least for a beginner. ARGOS is not designed to handle “Cold-war” scenarios like the one at Bodø in this report and produce questionable results in this case.

DEGADIS gives the user good control over the input parameters since each parameter has to be set during a sequence of question from the program. DEGADIS has default values for each parameter that can be used, if desired, but a relatively high user competence is necessary. The simulation starts by generating an input-file with the selected input parameters. Changes could easily be made in the input file without going through the whole input sequence mentioned above. The simulations are quite fast. It is not sure that the first run gives the desired output in terms of temporal and spatial scales. It might be desirable to re-run the program with new values in the input-file, for instance to investigate the maximum downwind propagation of the plume. DEGADIS does not have its own graphical user interface; this means that the numerical output must be imported into other programs, like MATLAB or Excel to produce a graphical plot. It is also a disadvantage that DEGADIS does not handle different terrain, a flat surface is assumed. It is, however, possible to define the surface roughness. DEGADIS is not suitable to handle releases of chemical warfare agents and non-heavy gases.

8 Conclusions

The hazard prediction and assessment tools, “Farlig gods” (from DSB) and ERGO are simple and give quick answers. The tools are easy to use, and can be used by non-experts. The “Farlig gods” program is mainly a database containing information about hazardous materials, their properties, and safety precautions. The possibility to calculate the safety distance for some of the chemicals in the database is only an extra functionality which, according to DSB, should be used with caution. Only the vapour pressure of the agent at the actual temperature is used to recommend a safety distance.

The initial isolation and protective action distances given by ERGO for each substance are on the other hand based on statistical evaluations and is well documented. These distances are given for small and large spills, and different results are obtained for releases during day- or night-time, respectively. ERGO partly accounts for the different meteorological conditions during day- and night-time. The software is designed for use at dangerous goods incidents occurring on a highway or railroad and should not be used for large releases.

The current version of NBC-Analysis (from Bruhn NewTech), uses ERGO to calculate the initial isolation and protective action distances for toxic industrial chemicals. It has some modifications to account for very large releases, which make this program more suited for large scale releases than ERGO. This will be even more elaborated in the coming version of NBC-Analysis which will be based on the new NATO ATP-45(D). For the release of chemical warfare agents, the results from NBC-Analysis are based on its own procedures. Here, many input parameters, both with respect to meteorology and the weapon used could be entered, if available. NBC-Analysis does not produce distances to specified concentration levels, only the area which is unsafe to enter. The safety distances are therefore regarded to be on the safe side and should be narrowed down if more detailed information on the extent of the contamination is known.

The Hazard Prediction and Assessment Capability (HPAC, from the U.S. Defense Threat Reduction Agency (DTRA)) is a comprehensive software tool which includes a chemical dispersion model. The program has been through extensive testing and evaluation and is used by many NATO countries. The program gives output data with relatively few input values, but then the results will be uncertain. To be able to obtain credible results, a lot of input from the user is necessary. The program has a high user entry level and a high degree of experience is required. It is also necessary to have meteorological data available, preferably on-line.

The Accident Reporting and Guiding Operational System (ARGOS, from Beredskapsstyrelsen (Danish Emergency Management Agency, DEMA), Risø National Laboratory and Prolog Development Center) is a flexible program. The chemical module is relatively new and still under development, and still has some irritating bugs. ARGOS is an open source software, where all the consortium members can contribute in the development. A lot of input from the user is necessary in order to produce credible results. The program has a high user entry level and needs a high degree of experience by the users. It is also necessary to have meteorological data available, preferably on-line.

The DEnse GAs DISpersion (DEGADIS) program (from U.S. Environmental Protection Agency) gives the user good control with the input values, since the software guides the user sequentially through an input sequence. The program is quick to use, but it might be necessary to do several runs to get the desired output. DEGADIS has no graphical output and the plots need to be performed using external programs. The program is designed to handle dense gases, and is not suitable for lighter-than-air industrial chemicals or chemical warfare agents. The program also has a high user entry level and a high degree of experience is required by the users.

The “Farlig gods” program and ERGO are both simple in use and can quickly be used by relatively inexperienced users when a release has taken place. They only provide information about areas where protective actions should be considered. Of these two programmes, ERGO is the most advanced and best documented, while “Farlig gods” gives more information on the properties of the material. NBC-Analysis gives no safety distances based on quantitative hazard levels, but produce an area which is unsafe to enter, and should therefore be on the safe side, i.e. produces larger danger areas than HPAC and ARGOS.

HPAC and ARGOS give relatively equal results from the release of chlorine at Ørland MAS, when the release is over land. When the release is over water, ARGOS gives larger hazard areas compared to HPAC. When used on the ammonia release at Kjeller, ARGOS produces larger hazard areas then HPAC. DEGADIS is designed to handle dense gases and, for chlorine, predicts a longer travel distance of the cloud than ARGOS and HPAC and a lower vertical spread than HPAC. It was not possible to get results for all the ammonia vignettes, and DEGADIS is therefore not included for this scenario. DEGADIS may not be suited for the release of ammonia anyway, because ammonia is lighter than air, at least some distance from the release. Neither ARGOS, nor DEGADIS are suited to handle an aerial attack and subsequent release of chemical warfare agents, like the one we have simulated at Bodø MAS. HPAC gives in this scenario a smaller area as compared to NBC-Analysis, which is in agreement with the idea that NBC-Analysis should produce an area based on worst-case thinking.

HPAC and ARGOS include source term modules. The evaporation rates from a pool of ammonia and chlorine were calculated and compared with a calculation with formulas for pool evaporation from the TNO Yellow Book. There were large discrepancies between the results, and this will in turn influence the dispersion modelling.

No exact solutions to the geographical dimensions of the contaminated area from a release of toxic industrial chemicals or chemical warfare agents could be given before the actual release has taken place. The results from the evaluated programmes have large uncertainties, and will only give guidance to the dangerous areas. Only real measurements on site after the release has taken place will reveal the true contaminated area. The programmes could be used to estimate the area affected and the probable number of affected people. It is, however, more difficult to estimate the exact position of the affected area due to uncertainties and constant variations in the wind direction. The meteorological conditions will vary with height above ground and with the distance from the release point. It is therefore important to have meteorological data for several positions throughout the computational domain in order to predict the hazard area as correctly as possible.

For the programs HPAC, ARGOS and DEGADIS, the user needs detailed input of the release, for example amounts of material released, outlet geometry of the container from which the agent is released and meteorological conditions. All these parameters could be difficult to obtain in a real situation. These programs are not suited for operational use by personnel with limited training on the software. They are, however, well suited for training and exercises to test different release scenarios before the release take place in order to learn more about the release of toxic chemicals. In addition, one could have ready pre-prepared scenarios where only changes in meteorological conditions and released amounts are entered before use. This will make it easier to do the assessment fast when there is a need.

The main conclusions of this study are:

- The box model for heavy gases (DEGADIS) and the Gaussian dispersion models which are included in two decision support systems (HPAC and ARGOS) give large variations in calculated plume prediction patterns for the three scenarios. Not all programs are suited for all scenarios. Hence, decisions based solely on the use of one of these programs can lead to serious misjudgements. It is important to have several models available and to know which model to employ for a given scenario. FFI will continue to test and evaluate these and possible other models for other scenarios.
- A fairly high user competence level is required for HPAC, ARGOS and DEGADIS.
- When HPAC or ARGOS is used in an operation or in a crisis situation, a real-time connection to a meteorological service is highly desirable.
- The "Farlig gods" program and ERGO are both simple to use, even for inexperienced users. They only give areas where protective actions should be considered. NBC-Analysis gives no safety distances based on quantitative hazard levels, but produces an area which is considered unsafe to enter.

An important weakness of the present work is the lack of experimental data for the dispersion of toxic industrial chemicals in selected reference scenarios, obtained either from field trials or wind-tunnel experiments. Due to the lack of experimental results, the comparison of results is only relative; since measurements are not available, we can not conclude which of the software packages that give results closest to observations. There is an urgent need for well-defined experimental measurements of dispersion of toxic chemicals in various types of topographies which can be employed in dispersion model development, inter-comparison and validation. FFI is contributing to pursue this goal through an ongoing collaboration with the Naval Surface Warfare Center which also includes participation in field experiments on large releases of ammonia and chlorine financed by the U.S. Department of Homeland Security. Also, FFI is taking initiative to launch a new project under the European Defence Agency (EDA) with the objective to establish a database of high-fidelity numerical simulations and experimental data from measurements of dispersion of dense gases in complex urban geometries.

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