A methodology to prioritise substances for possible further development of Acute Exposure Threshold Levels (AETLs)

Prepared by the **Health and Safety Laboratory**
for the Health and Safety Executive 2006

RESEARCH REPORT 426

HSE
Health & Safety Executive

A methodology to prioritise substances for possible further development of Acute Exposure Threshold Levels (AETLs)

Mary Trainor PhD BSc
Ron W Macbeth BSc A
Jill Wilday BSc
Helen F Balmforth PhD BSc
Health and Safety Laboratory
Harpur Hill
Buxton SK17 9JN

Peter Ridgway BSc
Health and Safety Executive
Redgrave Court
Merton Road
Bootle
Merseyside L20 7HS

The aim of the Acute Exposure research project, ACUTEX, is to develop a methodology for establishing European Acute Exposure Threshold Levels, AETLs, for toxic substances in relation to harm to people by inhalation. The development of AETLs is initially in the context of the risks of major accidents from chemical sites and in particular their regulation through the EU 'Seveso II' Directive. It is intended that AETLs can be used within Member States, where appropriate, to inform decisions on land-use planning and emergency planning.

This report describes the development of a prioritisation methodology to inform initial substance selection for a possible further AETLs programme. The work was based on consultation with experts drawn from EU major stakeholder groups. It included a Validation Exercise working with 3 Member States which account for between approximately 40% and 50% of all EU Seveso II sites. From this Validation Exercise we infer that, if these three Member States are representative in terms of numbers of priority substances, then the number of EU higher priority substances for further AETLs development is unlikely to be much in excess of 50.

This report and the work it describes was co-funded by the Health and Safety Executive (HSE) and the EU's Fifth Framework Programme of Research. Its contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.

HSE BOOKS

First published 2006

ACKNOWLEDGEMENTS

We are grateful to all the Critical Review Panel members and the researchers in the ACUTEX project who have contributed to the development of these substance prioritisation schemes. Particular thanks go to Maureen Wood, MAHB, who liased with Competent Authorities and EU stakeholders to clarify various issues on our behalf, to Pasquale Avino and Mauriziano Manigrasso of ISPESL who provided information on behalf of the Italian Competent Authority, to Ghislaine Verrhiest of the Ministere de L'Ecologie et du Developpement Durable who provided information on behalf of the French Competent Authority, and to our HSE and HSL colleagues who have contributed to or advised on this work: Graham Atkinson, Dave Bosworth, Dave Carter, Eliot Deag, Ian Hirst, Steve Porter, Stuart Reston, Ralph Rowlands, and Dave Webber.

CONTENTS

Executive Summary

Background: The ACUTEX Project

The aim of the Acute Exposure project, ACUTEX, is to develop a methodology for establishing European Acute Exposure Threshold Levels (AETLs) for toxic substances in relation to harm to people by inhalation. At this stage, their development is in the context of the risks of major accidents from chemical sites and in particular their regulation through the EU Seveso II Directive. As part of the development of the methodology, AETLs are being developed for 21 case-study substances. One possible outcome following the ACUTEX project is an EU program of AETLs development.

Objectives for Substance Prioritisation and Research Method

As part of the ACUTEX project, the Health and Safety Laboratory worked with the Health and Safety Executive to develop a prioritisation methodology to inform the selection of further substances for AETLs development following the ACUTEX project, if an AETLs program goes ahead. The work was based on consultation with experts from the major EU stakeholder groups. The development of the prioritisation methodology included a Validation Exercise working with 3 Member States which account for between approximately 40% and 50% of all EU Seveso II sites.

Main Findings

1.The Issue for Prioritisation
The issue for prioritisation is: 'What is the most cost-effective choice of substances for AETL development in order to reduce off-site risk/hazard to the public from major accidents at Seveso II sites, given that it is intended that AETLs can be used within Member States, where appropriate, to inform decisions on emergency planning or land-use planning?' Addressing this issue requires: identifying substances for which the off-site risk/hazard to the public is greatest; and taking account of EU policy issues and value for money considerations.

2. The Scope of Substances
The Critical Review Panel is advising the EU Commission on the scope of substances for inclusion in any further AETLs program. (Our role has been to advise the Critical Review Panel on supporting scientific and technical issues.) The scope the Critical Review Panel is advising at this time is based on the Seveso II Directive, but additionally encompasses other substances identified by Competent Authorities as being of particular interest in terms of off-site risk/hazard. It may be summarised as substances which are: Toxic, Very Toxic, Named Carcinogens in the Seveso II Directive, Corrosive or Irritant. Additional categories of substance may also be considered to be in-scope of the basis of expert judgment.

3. The Hazard Measures Used to Rank Substances According to Their Potential for Off-Site Harm

In the prioritisation methodology, one of the criteria used to rank substances is their potential to cause off-site harm based on substances' inherent properties and potential release tonnage during a hypothetical accident at a site. It was not possible to base prioritisation on an assessment of risk defined by objective measures of both hazard and exposure potential because information on exposure potential is not readily available. For substances which are Named

Carcinogens, ranking is done on the basis of expert judgment, while for Toxic, Very Toxic, Corrosive and Irritant substances it is done using quantified `hazard measures'. The hazard measures allow fluids (liquids and gases) to be ranked relative to one another, and solids to be ranked relative to one another. The relative ranking of fluids and solids is done on the basis of expert judgement. For both fluids and solids there are two hazard measures. The first hazard measure gives a rough indication of the relative potential for off-site harm posed by substances independent of release quantity, that is to say determined solely on the basis of their inherent properties. The second hazard measure gives a rough indication of the relative potential for off-site harm taking potential release quantity into account.

For fluids the two hazard measures give the area in km^2, which would be covered by a plume for a hypothetical catastrophic release from a site together with supplementary information on the plume downwind extent. The area and downwind extent are for the plume's $4hLC_{50}$ footprint, that is to say, the extent of the plume within which the concentration can exceed the $4hLC_{50}$. For solids, the first hazard measure is to prioritise according to $1/4hLC_{50}$: that is to say the lower the $4hLC_{50}$ the greater the toxicity. This is based on the potential for solids to be dispersed off-site in fires (for example warehouse fires). The second measure is to prioritise according to increasing: release quantity/$4hLC_{50}$.

At this time, information on potential release quantities is not readily available from Competent Authorities. Therefore, the potential release quantities considered for the hazard measures are the threshold site tonnages specified in the Seveso II Directive for `top-tier' (Article 9) sites and `lower-tier' (Articles 6 and 7) sites. In line with this, Competent Authorities are asked to identify whether their nominated substances contribute significantly to the risk/hazard for `top-tier' sites, or contribute to the risk/hazard from any Seveso II sites.

4. The Prioritisation Methodology

The prioritisation methodology may be broadly summarised as follows. Prioritisation of a substance is independent of the availability of toxicological data or the existence of other thresholds.

i) Member State Competent Authorities nominate substances, consulting stakeholders at national level as appropriate. They identify which of their nominated substances contribute significantly to the off-site risk/hazard from top-tier Seveso II sites, referred to as the 'higher priority substances', and which substances contribute to the off-site risk/hazard from any Seveso II sites, referred to as the 'lower priority substances'. For Corrosives and Irritants, they provide potential site release tonnage and, optionally, an indicative priority (higher or lower). Optionally, each Competent Authority also indicates: the number of sites for which the risk/hazard is dominated by each nominated substance; and whether there are any specific prioritisation factors at a national level which they wish to have taken into account.

ii) Those nominated substances which are in scope are assigned to the preliminary higher priority and lower priority substance lists. For Corrosives and Irritants this is done according to their potential to cause off-site harm using the hazard measures. Within the preliminary higher and lower priority substance lists, the substances are ranked according to the number of Member State nominations, together with the substances' potential to cause off-site harm using the hazard measures. Optionally, the number of sites for which the risk/hazard is dominated by these substances may be used as a 'tie-breaker' where substances have a similar rank. Any additional national-level prioritisation factors raised by Competent Authorities are taken into account on a case-by case basis. Ranking of the preliminary higher and lower

priority substance lists is independent. Together with consideration of any EU policy issues, this gives a preliminary EU higher priority and lower priority list of substances for AETLs development for consultation purposes.

iii) Proceeding in parallel with ii.), nominations are checked and additional supporting information is requested from Competent Authorities if necessary.

iv) Following EU-level stakeholder consultation, and taking into account the costs and benefits of AETLs development, a first list of substances for AETLs development is decided. This first list might, for instance, comprise: the higher priority substances with greatest rank; or all the higher priority substances; or all the higher priority substances together with the lower-priority substances of greatest rank.

v) AETLs are developed. During this time, the list of substances for AETLs development is kept under review according to changing stakeholder needs.

At this time, the relative importance in the ranking process of the number of Member State nominations and the hazard measures for a substance has not been decided. This is a policy matter left for consideration by the Competent Authorities.

5. The Need for Further Stakeholder Consultation

In the event that a program of further AETLs development is agreed, the methodology will be subject to further stakeholder consultation. This is to allow the methodology to be updated as necessary to take into account factors such as the money which will initially be made available for AETLs development (which in turn will affect the number of substances to be selected), and any changes to stakeholder priorities or data availability. For example, if the money initially available for an AETLs program would only cover higher priority substances, then initial Member State nominations might be invited for these substances alone. Equally, ranking of the higher priority substances may be unnecessary if the funding would cover AETLs development for all of them. Similarly, any changes to data availability would need to be taken into account. For instance, if information on potential release tonnages were in future available (for example, expressed as typical tonnages of concern for a substance) the methodology could be modified accordingly.

6. Indication of Number of Further EU Priority Substances

During the Validation Exercise the Competent Authorities for the three participating Member States, France, Italy and the UK, proposed 141 further in-scope substances for AETLs development. Of these 141 substances, 19 are higher priority and 134 are lower priority. We infer that, if these three Member States are representative in terms of numbers of priority substances, then the number of EU higher priority substances for further AETLs development is unlikely to be much in excess of 50.

7. Technical Support

The technical support which will be required for AETLs substance prioritisation includes: information on substance inherent hazardous properties; a database on nominated substances; and a password protected website for access by Competent Authorities and major EU stakeholder groups.

1 INTRODUCTION

1.1 THE ACUTEX PROJECT AND ACUTE EXPOSURE THRESHOLD LEVELS, AETLS

The aim of the Acute Exposure project, ACUTEX, is to develop a methodology for establishing European Acute Exposure Threshold Levels (AETLs) for toxic substances in relation to harm to people by inhalation. At this stage, their development is in the context of the risks of major accidents from chemical sites and in particular their regulation through the Seveso II Directive. A broader future context has not been precluded. It is intended that AETLs can be used within Member States, where appropriate, to inform decisions on land-use planning and emergency planning.. It is intended that AETLs will be complementary to US Acute Emergency Guideline Levels (AEGLs) while meeting needs specific to European users. As part of the development and testing of the methodology, AETLs are being produced for 21 case study substances. One possible outcome following the ACUTEX project is an EU program of AETLs development.

The work of the ACUTEX project is being monitored by a Critical Review Panel comprising experts from major EU stakeholder groups including emergency planners, industry, Competent Authorities (the EU Member State enforcing authorities for the Seveso II Directive), toxicologists, and risk-related decision makers. The Critical Review Panel is chaired by the European Commission's Major Accident Hazards Bureau, MAHB.

Appendix 1 gives further details of the ACUTEX project and Appendix 2 gives details of the US AEGLs program.

1.2 SUBSTANCE PRIORITISATION FOR AETLS DEVELOPMENT

As part of the ACUTEX project, the Health and Safety Laboratory (HSL) worked with the Health and Safety Executive (HSE) to develop two prioritisation methodologies to inform the selection of substances for which toxicity thresholds will be developed:

- The first prioritisation methodology informed the selection of 21 preliminary substances for use by ACUTEX toxicologists as AETL case studies. This methodology focused on meeting the scientific needs of the toxicologists and the selection was based on lists of '10 Substances of Interest' proposed by Member State Competent Authorities [Trainor et al., 2003] and [Trainor et al., 2004].

- The second prioritisation methodology is to inform the selection of further substances for AETLs development following the ACUTEX project if an AETLs program goes ahead. This methodology focuses on determining how to make the most cost-effective choice of substances for AETLs development in order to reduce off-site risk/hazard to the public from Seveso II sites. It is the subject of this report.

1.3 THE STRUCTURE OF THIS REPORT

Chapter 2 describes the approach we used to develop the prioritisation methodology for possible further AETLs development, the issue for prioritisation and the requirements we aimed to address.

Chapter 3 describes the scope of substances for further AETLs development, which is being advised at this time by the Critical Review Panel.

Chapter 4 describes the practical considerations that to some extent dictated the prioritisation methodology. These include data availability at EU and Member State level, and commonalities in implementing the Seveso II Directive across the EU.

Chapter 5 describes the prioritisation methodology. There are 6 criteria (1 for substance selection and a further 5 for ranking purposes) which, together with consideration of policy issues are used to draw up an EU preliminary higher priority list and lower priority list of substances for AETLs development based on substances nominated by Member States. The lists are then used to inform the selection of an EU first list of substances for AETLs development taking into account stakeholder consultation, and value for money considerations. We give a flowchart showing how the different aspects of AETL prioritisation fit together.

Chapter 6 gives the technical details of the hazard measures used to rank substances according to their potential to cause off-site harm.

Chapter 7 summarises the outcome of a Validation Exercise, which we carried out working with the Italian, French and UK Competent Authorities. The chapter discusses the significance of the numbers of higher and lower priority substances nominated. In particular, we infer that if these three Member States are representative in terms of numbers of priority substances, then the number of EU higher priority substances for further AETLs development is unlikely to be much in excess of 50.

Chapter 8 outlines the technical support, which we suggest will be needed for substance prioritisation. This includes: information on substance hazardous properties; a substance database; and a website for access by Competent Authorities.

Finally Chapter 9 describes how the prioritisation methodology relates to the prioritisation requirements identified in Chapter 2, taking into account the technical support requirements we have suggested.

2 DEVELOPMENT OF THE PRIORITISATION METHODOLOGY FOR POSSIBLE FURTHER AETLS DEVELOPMENT

Below we describe: the approach we used to develop the prioritisation methodology for possible further AETLs development; the overall aim in developing the prioritisation methodology; the issue for prioritisation; the requirements for the prioritisation methodology; and our remit. Additionally, Appendix 4 gives an overview of some approaches to substance prioritisation adopted elsewhere: this material provided us with helpful background for the development of the AETLs substance prioritisation methodologies.

2.1 APPROACH TO DEVELOPMENT OF THE PRIORITISATION METHODOLOGY FOR POSSIBLE FURTHER AETLS DEVELOPMENT

We sought the views of the major European stakeholders represented on the ACUTEX Critical Review Panel, the ACUTEX partners, and the ACUTEX Steering Committee at each stage of the methodology's development. This was in order to ensure that their priorities and the significant factors of importance they identified, were fully addressed in the final methodology.

Our development of both the prioritisation methodology for possible further AETLs development, and the earlier prioritisation methodology which was used to inform the selection of the 21 case study substances, was underpinned by a stakeholder consultation exercise conducted at the outset to identify 'factors of importance' for prioritisation. The aim was to:

- give a basis for substance prioritisation criteria;
- clarify the separate aims of the two prioritisation schemes; and
- clarify our remit.

The stakeholder consultation exercise was initiated and coordinated by MAHB acting as chair of the Critical Review Panel. This elicited the views of the major European stakeholders represented on the ACUTEX Critical Review Panel (we received anonymised views); and of EU Competent Authorities and EU Candidate States. This was an iterative process in which we sought clarification of responses via MAHB as coordinator. We note that stakeholder views included those of CEFIC, The European Chemical Industry Council, following a workshop they held on ACUTEX during which a number of factors of importance were proposed. Also, HSE consulted UK stakeholder groups including emergency planners, academics and industry.

An important need in development of the prioritisation methodology for further AETLs development was to establish an indication of the number of EU priority substances and the degree of consensus on these substances between Member States, since this determined the degree of complexity needed. It was also important that the methodology used information that could be readily supplied by Competent Authorities. We therefore carried out a Validation Exercise working with the French, Italian and UK Competent Authorities which considered both data availability and numbers of substances. As part of this Validation Exercise, we hosted a Validation Workshop attended by representatives from the French, Italian and UK Competent Authorities, the chair of the ACUTEX Critical Review Panel, and a representative of the steering committee for the ACUTEX project.

In the event that a program of further AETLs development takes place, the methodology will be subject to further stakeholder consultation. This is to allow the methodology to be updated as necessary to take into account factors such as the money which will initially be made available for AETLs development (which in turn will affect the number of substances to be selected), and any changes to stakeholder priorities or data availability.

2.2 THE OVERALL AIM IN DEVELOPING THE PRIORITISATION METHODOLOGY

The overall aim was to develop a prioritisation methodology that facilitates both the decision making process and its transparency by providing a common, agreed framework. This is within the context of the principles in the European Commission White Paper on Risk Governance [European Communities. Commission, 2001] including the need for openness and the fair treatment of all Member States. A discussion of risk analysis within regulatory decision-making, based on a workshop held at the European Commission's Joint Research Centre, is given in [Otway & Peltu, 1985].

2.3 THE ISSUE FOR AETLS SUBSTANCE PRIORITISATION

For further AETLs substance prioritisation, the issue, as confirmed by the initial consultation exercise with major EU stakeholders, is:

> 'What is the most cost-effective choice of substances for AETL development in order to reduce off-site risk/hazard to the public from major accidents at Seveso II sites, given that it is intended that AETLs can be used within Member States, where appropriate, to inform decisions on emergency planning or land-use planning?'

Addressing this issue requires:

1.) identifying substances for which the off-site risk/hazard to the public is greatest;
2.) taking account of EU policy issues, and value for money considerations; and
3.) consulting stakeholders.

The need to address policy and value for money issues and to further consult stakeholders is highlighted in the prioritisation methodology. An example of an EU policy issue which may need to be taken into account is possible international collaboration by the EU on toxicological databases used to underpin threshold development.

We note that the issue for AETLs prioritisation is expressed in terms of off-site risk/hazard since across the EU Member States a range of hazard and risk based approaches are used in the control of major accident hazards as regulated through the Seveso II Directive. For example, a description of the various approaches and criteria applied in EU Member States for land-use planning purposes is given in [Christou et al., 1999].

2.4 REQUIREMENTS FOR CRITERIA FOR AETLS SUBSTANCE PRIORITISATION

The main requirements for the prioritisation methodology and criteria are:

Requirement 1.)	The criteria are acceptable and transparent to EU major stakeholders.
Requirement 2.)	The criteria use information which can be readily supplied by Competent Authorities.
Requirement 3.)	The methodology and criteria are designed to minimise the cost associated with prioritisation by using the simplest approach and by making the minimum information demands on Competent Authorities consistent with meeting requirement 1.
Requirement 4.)	The methodology is flexible so that it can be adapted to changing needs. For example, under ACUTEX: • AETLs development is restricted to the context of chemical sites and specifically the Seveso II Directive, however a broader future context has not been precluded; and • AETLs development is restricted to the toxicity of individual substances because of the uncertainties in the knowledge of the toxicity of mixtures, however consideration of the effects of mixtures of substances might be technically feasible at a future date.
Requirement 5.)	Where practicable, the methodology should draw on, or complement methodologies, criteria, and information collected from Member States through other Seveso II programs or projects.
Requirement 6.)	The methodology should be of a level of detail appropriate to the task, in particular taking into account how many substances are likely to need to be prioritised.

In Chapter 9 we discuss how we consider these requirements have been met.

2.5 OUR REMIT IN DEVELOPING THE PRIORITISATION METHODOLOGY FOR POSSIBLE FURTHER AETLS DEVELOPMENT

Our remit was to develop a prioritisation methodology based on criteria that are, so far as is possible, objective. This takes into account that applying scientific and technical criteria may require a degree of expert judgement. Additionally, our remit was to advise the Critical Review Panel on technical and scientific issues underpinning their advice on the scope of substances for AETLs development.

Our remit did not include considering EU policy issues or value for money considerations. In particular, our remit did not include considering the ‘cut-off’ which will be used to determine which priority substances will be included in the first list of substances for AETLs development. Addressing the latter will entail considerations such as value for money, and will be informed by the outcome of ACUTEX.

3 THE SCOPE OF SUBSTANCES FOR POSSIBLE FURTHER AETLS DEVELOPMENT

3.1 THE SCOPE OF SUBSTANCES BEING ADVISED AT THIS TIME BY THE CRITICAL REVIEW PANEL

The ACUTEX Critical Review Panel consists of a Panel of experts representing a number of stakeholder interests including end-users and scientific organisations, industry and competent authorities, and local and national levels. It is intended to offer a cross-section of technical perspectives that will help improve acceptance and usefulness of the methodology within Europe. Its advice takes into account technical and scientific issues, including how certain aspects affect the practicality and flexibility of outcomes for decision-makers. In this role, the Critical Review Panel also advised the project on a scope of substances for possible further AETLs development within the context of control of major industrial hazards and in particular their regulation through the Seveso II Directive. Our role has been to advise the Critical Review Panel on technical and scientific issues. Appendix 5 gives background information on:

- the EU classification of dangerous substances including the use of risk phrases and classification in Annex 1 of the Dangerous Substances Directive (the 'Annex 1' Classification); and
- the coverage of dangerous substances by the Seveso II Directive.

At this time, the Critical Review Panel is advising a scope which is based on the Seveso Directive but which additionally encompasses other substances identified by Competent Authorities as being of particular interest in terms of off-site risk/hazard to the public from chemical sites. The scope covers individual substances only. Mixtures of substances are out of scope because of the scientific limitations on the thresholds that toxicologists can currently develop. The importance of mixtures in terms of off-site risk due to the possibility of, for instance, synergistic effects, is recognised.

The scope which the Critical Review Panel is advising at this time may be summarised as substances which are:

Toxic, Very Toxic, Named Carcinogens in the Seveso II Directive, Corrosive or Irritant.

In detail, the scope being advised is in three parts as follows.

3.1.1 Scope Part 1: Substances Covered by the Seveso II Directive in Terms of their Acute Toxicity

These substances are as follows:

1a) the Named Carcinogens in Part 1 of the Seveso II Directive;
1b) all other Named Substances in Part 1 of the Seveso II directive which are classified as either Toxic with the risk phrase R23, R24, R25 or R39, or Very Toxic with the risk phrases R26, R27 or R28; and

1c) substances in the categories of either Toxic with the risk phrases R23, R24, R25 or R39, or Very Toxic with the risk phrases R26, R27 or R28 under Part 2 of the Seveso II Directive.

Note that the EU classification category of Toxic also includes substances with R48, assigned on the basis of toxicity following repeated exposure. Substances classified as Toxic solely because the criteria for R48 are met are considered to be out of scope because such substances lack the appropriate acute toxicity properties.

We note that the majority, that is 88% (143 out of 162) of the in-scope substances nominated by the 3 Competent Authorities involved in the Validation Exercise were in scope as defined here under Scope Part 1.

3.1.2 Scope Part 2: Toxic and Very Toxic Substances Misclassified under Annex 1 of the Dangerous Substances Directive

For some substances, the Annex 1 classification with respect to the Toxic and Very Toxic categories is inconsistent with the currently available toxicity data. We refer to these substances as 'misclassified'[1]. In such cases the classification determined by a competent toxicologist based on a review of all the currently available toxicity data will be used in preference to the Annex 1 classification to determine whether a substance is in scope for AETLs development.

We note that about 11% (about 18 out of 162) of the in-scope substances nominated by the 3 Competent Authorities involved in the Validation Exercise, were considered to be in scope because they have acute inhalation toxicity data supporting a Toxic or Very Toxic Annex 1 Classification although they were not classified as such in Annex 1. We do not know how many nominated substances are likely to be found to be out of scope because they have a Toxic or Very Toxic Annex 1 Classification which is not supported by current acute inhalation toxicity data.

We stress that only those misclassified substances which have toxicity data supporting a Toxic or Very Toxic classification are considered to be in scope.

3.1.3 Scope Part 3: Corrosive and Irritant Substances

Substances which are classified as Corrosives or Irritants are in scope.

This is a pragmatic recommendation which allows the inclusion of substances whose toxicity is somewhat below that which would classify them as Toxic. (In other words, substances with an LC_{50} above the threshold for classification as Toxic.) A small number of these substances are of interest to Competent Authorities because they could potentially be released in very large quantities from a chemical site. Consequently, these substances can pose an off-site hazard/risk to the public which is considered by the Competent Authorities to be as significant as that from substances which come under the scope of the Seveso II Directive because of their acute

[1] The classification of individual substances in Annex 1 of the Dangerous Substances Directive is sometimes modified, for example following proposals by Member States. The accuracy of Annex 1 classifications is discussed by [Ruden and Hansson, 2003]. They note a lack of transparency in the classification decision-making process, particularly for substances classified in the early years of the current system, which means that the reasons behind some existing classifications are unclear.

toxicity. We note that less than 1% (1 out of 162) of the in-scope substances nominated by the 3 Competent Authorities involved in the Validation Exercise were in scope because they are Corrosive or Irritant.

3.1.4 Additional Considerations

The scope of substances for AETL will be kept under review. Also, additional categories of substances may be considered as in scope on the basis of expert judgement. For example, this might include those substances with data indicating a potential to induce cancer following a single exposure but which are not Named Carcinogens in the Seveso II Directive.

3.1.5 The Potential for a Broader Scope of Substances

The remit of the CCAs in advising on a scope of substances for possible further AETLs development is limited to the context of the risks of major accidents from chemical sites and in particular their regulation through the Seveso II Directive.

However, a wider scope of substances for further AETLs development has not been precluded. For example, areas of possible interest include pipelines and the transportation of dangerous goods.[2] If the scope of substances for AETLs development is widened, the substance prioritisation methodology would need to be extended accordingly.

[2] Additionally, further thresholds considering harm to the environment rather than to people, are of possible future interest in the context of the Seveso II Directive.

4 PRACTICAL CONSIDERATIONS INFLUENCING THE PRIORITISATION METHODOLOGY

Our development of the prioritisation methodology for possible further AETLs development was dictated to some extent by practical considerations of data availability at EU and Member State level, and commonalities in implementing the Seveso II Directive across the EU. Three direct consequences are that the methodology is based on the following:

- Priority Substance Lists nominated by individual Competent Authorities.
- Criteria which do not include estimates of off-site risk.
- Information from individual Competent Authorities on whether substances contribute significantly to the off-site risk/hazard from Seveso II sites, rather than detailed information on potential release tonnage and likelihood of release.

Additionally, practical considerations determined the basing of the prioritisation methodology on:

- Use of approximate $4hLC_{50}$ as an indication of relative toxicity in determining the potential of substances to cause adverse health effects for ranking purposes.

Further details are given below.

4.1.1 The Need to Use Competent Authorities' Priority Substance Lists

We considered whether it would be possible to avoid the use of priority substance lists from Member States by use of existing EU information on high-production tonnage substances[3]. We ruled out this possibility because:

- Substances which are not classed as high production can pose a significant off-site risk/hazard and may be considered as priority substances for AETLs development by Members States on this basis.
    - Firstly, a significant source of off-site risk/hazard is not production substances and their reaction products but rather intermediates and reagents etc.
    - Secondly, factors determining off-site risk/hazard include the inherent properties of a substance, how much can potentially be released from a site, and the size of the population in the vicinity of a site. This means that a substance which is not classed as high-production can pose a significant risk/hazard.
- By using Member States priority lists as a starting point, Member States priorities will be directly reflected in the final EU priority substance list for AETLs development.

We also note that the EU Seveso Plants Information Retrieval System, 'SPIRS' (see [European Communities, 2002]) holds information on numbers of sites for the Named Substances and Generic Categories of Substances as defined in the Seveso II Directive. However, because SPIRS is based on the requirements of the Seveso II Directive, the information is not broken

[3] Tonnage details for EU high production substances are held in The International Uniform Chemical Information Database (IUCLID) described in [Heidorn, 1996].

down by substance within the Generic Categories. Therefore, it does not provide sufficient information for AETLs substance prioritisation.

Additionally we considered a suggestion that instead of taking EU information as a starting point, the list of substances for AETLs development could be based on lists of substances for which other thresholds have been developed. The other thresholds suggested include those which can be used in the context of off-site risk from chemical plant such as US 'AEGL' [Rusch et al., 2000], US 'IDLH' [Alexeeff et al., 1989] and US 'ERPG' [Rusch, 1993] thresholds and those developed specifically for occupational exposures. In our view, the disadvantage of this approach is that it would neither identify those substances which are of most relevance within the EU in the context of off-site risk from chemical sites[4], nor reflect Member State priorities.

4.1.2 Use of Prioritisation Criteria Which do not Include Estimates of Risk

We note that there are two reasons why we did not consider the prioritisation of substances according to a quantitative estimation of risk:

- There are no EU-wide measures or criteria in use for assessing off-site risk. Rather, Competent Authorities have adopted approaches in line with national regulatory frameworks and existing measures in relation to chemical plant.
- Even if such a measure did exist, the demands on Competent Authorities, that providing the necessary information would entail, would be wholly disproportionate to the task in hand.

A description of the different approaches and criteria applied in the EU to take into account major accident hazards for land-use planning purposes is given in [Christou et al., 1999]. This groups the approaches into three broad categories:

- 'risk based', that is to say based on the assessment of both consequences and likelihoods (frequencies) of possible event scenarios, with the approaches used in the Netherlands and the UK described as examples;
- 'consequence based', that is to say based on the assessment of the consequences from the conceivable accidents without quantifying their likelihood, with the approach used in France described as an example; and
- based on establishing 'generic distances', that is to say safety distances derived usually from expert judgment and mainly based on historical reasons, with use in Germany and Sweden cited as an example. [Christou et al., 1999] also notes that in Germany the criteria 'are such that the installation should be established and operated so that no risk is imposed to man or the environment outside'.

We also note that the European Technical Working Group on Land-Use Planning ('TWG-5'), established in 2002, is currently developing a technical database of risk and hazard assessment data, including the consideration of a commonly agreed definition of risk-related indices and measures.

[4] For example, as part of the prioritisation of 21 preliminary substances for ACUTEX case studies [Trainor et al., 2003] ten Member State Competent Authorities nominated 39 substances of interest which were within the scope of substances for the case studies. About 10% of these substances were not on the US priority list for AEGLs development. We consider that this illustrates the need for an AETLs priority list to be based directly on EU priorities not those determined elsewhere.

It was also suggested by some representatives of the Critical Review Panel that prioritisation should be based on the definition of risk as hazard plus exposure potential. It should therefore include objective measures of both hazard and exposure potential. Such an objective measure of hazard is included in criterion R3. The project was unsuccessful at identifying a credible and easily obtainable measure of exposure potential. Several alternatives for measuring exposure potential or assigning surrogate measures were discussed including European production volume, quantity at Seveso sites, number of Seveso sites in Europe where it was present, and typical process location. Although some of these options may represent valid measures, these types of data are generally not centralised and therefore not readily available.

4.1.3 Use of Qualifying Quantities and Competent Authority Information on Substances' Contribution to Off-Site Risk/Hazard Rather than Potential Release Tonnage, and Likelihoods

In the prioritisation methodology, substances are ranked according to their potential to cause off-site harm, using:

- information from individual Competent Authorities on whether substances
    - contribute significantly to the off-site risk/hazard from top-tier (Article 9) Seveso II sites (these are considered to be 'higher priority substances'), or
    - contribute to the risk/hazard from any Seveso II sites (these are considered to be 'lower priority substances'); and
- 'hazard measures' derived from substances' inherent hazardous properties and Seveso II 'Qualifying Quantities'.

The exception is for Corrosive and Irritant substances since they are outside the scope of the Seveso II Directive. For these substances, the hazard measures use potential site release tonnage in place of Qualifying Quantities. The hazard measure is compared against those for other nominated substances to decide if they are to be considered as higher priority or lower priority substances.

These hazard measures are described in detail in Chapter 6 while Appendix 5 includes an overview of the coverage of dangerous substances by the Seveso II directive including the use of Qualifying Quantities to define lower-tier and top-tier sites.

Alternative approaches would be possible if data on potential release tonnages were readily available from Member State Competent Authorities. Industry representatives on the Critical Review Panel indicated a particular interest in having this information. However, Member State Competent Authorities hold only information appropriate to their regulation of chemical sites under the Seveso II Directive. Similarly, this information is processed and held at an appropriate level for regulation within that Member State. Therefore information on potential release tonnages is not at present held centrally in a readily available format. The latter was found to be the case during the Validation Exercise for the prioritisation methodology, and was confirmed by MAHB based on discussions with member States. (An example of one of the possible alternative ranking approaches is to rank substances according to the hazard measures using typical potential release tonnages of concern for substances nominated by Competent Authorities as being higher priority for AETLs development, and using Seveso II Qualifying Quantities for substances nominated as lower priority.)

The prioritisation methodology aims to use information which will be readily available to most Member States. We also note that, in our view, the available information is at an appropriate level for the purposes of substance prioritisation. However, substance nominations will be checked and, where appropriate, additional supporting information may be requested such as tonnage or information related to release likelihood.

4.1.4 Use of Approximate $4hLC_{50}$ as an Indication of Relative Toxicity in Determining the Potential of Substances to Cause Off-Site Harm for Ranking Purposes

For substances which are Toxic, Very Toxic, Irritant or Corrosive, the methodology uses approximate $4hLC_{50}$ as an indication of relative toxicity. (That is to say, the lower the $4hLC_{50}$ the greater the toxicity.) The use of approximate $4hLC_{50}$ for prioritisation purposes was decided on the basis that it is the best benchmark available to allow comparison and ranking of a list of diverse substances, and that it is fit for purpose in this context. We note in particular that the Seveso II Directive addresses potential off-site accidents in terms of both lethal and sub-lethal doses. By using approximate $4hLC_{50}$ we do not suggest or intend that prioritisation should be biased towards potentially lethal doses. For a discussion of the relationship between the risk of death, and the risk of being exposed to a sub-lethal dose, in the context of off-site risk from chemical plant, see [Franks et al., 1996].

A specific alternative suggested by one Critical Review Panel member was to use occupational Short Term Exposure Limits, STELs. This is because STELs have the advantage of representing the irritancy threshold for some substances and this threshold is likely to be a key toxicity endpoint for AETLs development. However, we found that significantly fewer STEL than approximate $4hLC_{50}$ values are available for the diverse substances of interest for AETLs development. In particular we considered their relative availability for the substances of interest for AETLs development which were initially proposed by Competent Authorities and used in the selection of the ACUTEX case study substances project. We found[5] that for the 39 substances within the scope of the ACUTEX case studies:

- 92% of substances have an approximate $4hLC_{50}$; whereas
- only 36% of substances have a specific STEL.

[5] STEL and approximate $4hLC_{50}$ values for each substance together with details of the databases we used are given in the spreadsheet in [Trainor et al., 2003].

5 THE PRIORITISATION METHODOLOGY AND CRITERIA FOR POSSIBLE FURTHER AETLS DEVELOPMENT

In this chapter we describe the prioritisation methodology and criteria for possible further AETLs development. Flowchart 5.1 shows how the different aspects of AETL prioritisation including substance nomination fit together. Figure 5.1 summarises the prioritisation criteria and illustrates how they link with the three other considerations for prioritisation: EU policy, stakeholder consultation, and value for money. This figure corresponds to Stages E, F and G of the flowchart.

The chapter first describes the flowchart, then the criteria summarised in the figure, and concludes with comments on the prioritisation methodology.

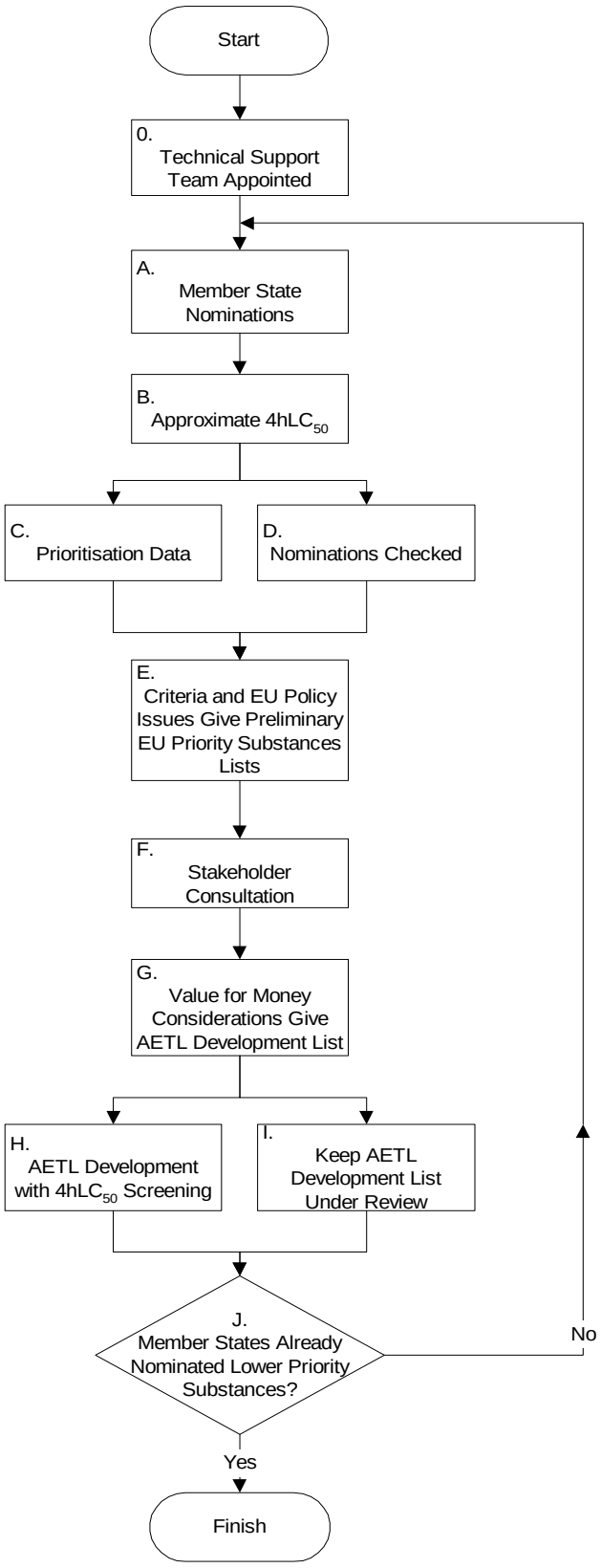
5.1 THE PRIORITISATION METHODOLOGY FLOW CHART

In this section we describe in detail the information shown in the flowchart on how the different aspects of AETL prioritisation fit together. The description of the flowchart assumes that the prioritisation process will involve these people:

- The AETL Selection Committee.
- A Technical Support Team providing technical information on substances nominated by Member States and handling most technical queries about nominations.
- Toxicological support on provision of approximate 4hLC_{50} information for substances for prioritisation purposes. This might best be done by the toxicologists who will be developing the AETLs. Alternatively it could be done within the Technical Support Team. The toxicologists would also advise on the relative potential for harm of any nominated Named Carcinogens if this is necessary in relation to criterion R3 (see below).

We stress the view of the Critical Review Panel that stakeholder consultation is fundamental to the prioritisation process. As well as the formal consultation stage included in the flowchart, the Critical Review Panel are recommending that there should be plenty of opportunity for consultation before and during the process.

Flowchart 5.1
Summary of How the Different Aspects of Prioritisation Fit Together



Criteria for All Nominated Substances		
Criterion	**Description**	
S1	In Scope: substance must be, Toxic, Very Toxic, Seveso II 'Named Carcinogen', or Corrosive/Irritant	
R1	Substance contributes *significantly* to off-site hazard/risk at top-tier sites: if yes, assign to preliminary higher priority list	Substance contributes to off-site hazard/risk at top- or lower-tier sites: assign to preliminary lower priority list

Criteria for Preliminary Higher Priority List	
Criterion	**Description**
R2	Give priority to substances nominated by more than one Member State
R3	Rank substances according to their relative potential to cause adverse health effects, based on physicochemical and toxicological properties and Seveso II Qualifying Quantity or Corrosives/Irritants site tonnage. Fluids: use modelled plume '4hLC_{50} footprint' Solids: use '1/4hLC_{50}'
R4 Optional	For substances with similar ranking, give priority to those dominating hazard/risk at greatest number of **top-tier** sites
R5	Take case-by-case account of additional factors raised by Member States

Criteria for Preliminary Lower Priority List	
Criterion	**Description**
R2	Give priority to substances nominated by more than one Member State
R3	Rank substances according to their relative potential to cause adverse health effects, based on physicochemical and toxicological properties and Seveso II Qualifying Quantity or Corrosives/Irritants site tonnage. Fluids: use modelled plume '4hLC_{50} footprint' Solids: use '1/4hLC_{50}'
R4 Optional	For substances with similar ranking, give priority to those dominating hazard/risk at greatest number of **lower-tier** sites
R5	Take case-by-case account of additional factors raised by Member States

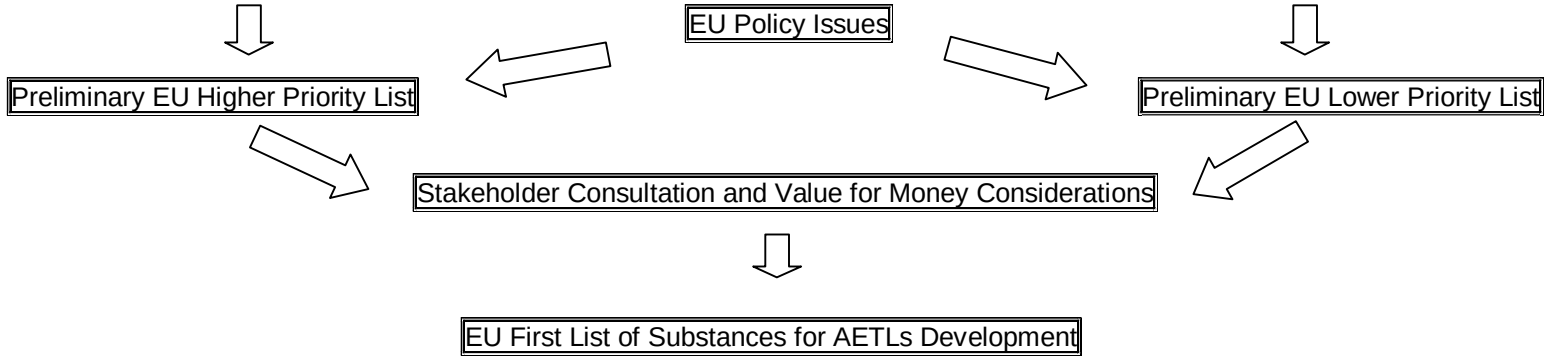


Figure 5.1: Summary of Proposed Criteria and other Considerations to be Applied to Substances Nominated by Member States, to Produce a Prioritised list of Substances for AETL Development

The description of the flowchart is as follows. The outcome is a first EU list of further substances for AETLs development.

0) Technical Support Team Appointed
Before prioritisation begins, the Technical Support Team is appointed and the provision of toxicological support on approximate $4hLC_{50}$ is agreed. The models to be used to determine substances' potential to cause off-site harm are agreed and a sensitivity analysis carried out (see section 6.3.2 below).

A) Member State Nominations
Prioritisation begins with the Member State Competent Authorities nominating their priority substances together with associated 'CAS' numbers from the Chemical Abstracts Service Registry. This is done in consultation with stakeholders at national level as appropriate. The information which the Competent Authorities supply is as follows.

- For those nominated substances which are Toxic, Very Toxic, or Seveso II Named Carcinogens, the Competent Authorities:
  - i.) identify which substances contribute significantly to the off-site risk/hazard from top-tier Seveso II sites, the 'higher priority substances';
  - ii.) identify which substances contribute to the off-site risk/hazard from top-tier or lower-tier Seveso II sites, the 'lower priority substances';
  - iii.) give a description of the information on which i) and ii) were based; and
  - iv.) optionally, give the number of sites for which the risk/hazard is dominated by each nominated substance, or other information on number of sites.

- For those nominated substances which are Corrosives and Irritants, the Competent Authorities give:
  - i.) the potential off-site release tonnage (this may be either typical tonnages of concern, or the potential off-site release tonnage for the worst-case site); and
  - ii.) optionally, an indicative priority (higher or lower).

- Optionally, the Competent Authorities indicate whether there are any prioritisation factors important at a national level which they wish to have taken into account.

- Optionally, the Competent Authorities identify any 'precursor' substances that they considered in identifying the nominated substances. These are substances which are NOT to be considered for AETLs development, but which are of interest because a nominated substance is a reaction product of one or more precursor substances[6].

Here, a top-tier site is one subject to Article 9 of the Seveso II Directive, that is to say on the basis of the higher Qualifying Quantities listed in Annex 1 of the Directive. A lower-tier site is one which is not subject to Article 9 and is regulated on the basis of the lower Qualifying Quantities listed in Annex 1 of the Directive. We note that in implementing the Seveso II Directive, some Member States have chosen to lower the Qualifying Quantities for some substances. It will therefore be necessary to stress to Competent Authorities that nominations must be on the basis of the Qualifying Quantities in the Seveso II Directive. The AETLs Selection Committee may decide initially to invite nominations of higher priority substances only and draw the first AETLs development list from these nominations.

[6] Several precursors were identified by the Competent Authorities involved in the Validation Exercise. We found that in the interests of transparency it was helpful to list these, even though they are not candidates for AETLs development.

B) Approximate 4hLC$_{50}$

The toxicologists then provide an approximate 4hLC$_{50}$ for each nominated substance. The approximate 4hLC$_{50}$ is needed to check whether the substance is in scope (criterion S1 described in section 5.2.1 below) and to generate the hazard measures (used for criterion R3 described in section 5.2.4 below). Because there is no standardised list of internationally accepted 4hLC$_{50}$ values, a database from an EU Member State could be used as the primary source of this information[7].

C) Prioritisation Data

The information needed for each substance in order to apply the prioritisation criteria is provided by the Technical Support Team. This includes checking the potential for use of a parameterised hazard measure for fluids prior to starting on the preliminary lower priority list (see section 6.3.3 below).

D) Nominations Checked

In parallel with C), nominations are checked. If the basis for nomination of a substance is unclear, the Technical Support Team liaise with the Competent Authority. This may entail asking for additional supporting information such as potential release tonnage for the worst-case site (in terms of off-site hazard/risk), or information linked to likelihood of release such as how a substance is being used, or could otherwise potentially be released from a site[8].

Similarly, where expert judgment will be needed to determine whether a substance is in scope for AETLs development, the nominating Competent Authority will be asked to provide supporting details. (As described in Chapter 3, although a defined scope will form the basis for most decisions on whether substances are in-scope, additional categories of substance can be considered on a case-by-case basis using expert judgment.)

The nomination checking process will include consideration of the numbers of Seveso II sites in each Member State. (This information is held in the EU Seveso Plants Information Retrieval System, 'SPIRS', see [European Communities, 2002].)

E) Criteria and Policy Issues Give Preliminary EU Priority Substance Lists

The AETLs Selection Committee, with assistance from the Technical Support Team and toxicologists as necessary, apply the 6 prioritisation criteria. Additionally, the AETLs Selection Committee addresses any policy issues which may affect prioritisation. The outcome is:

- a preliminary list of EU higher priority substances ranked in order of priority; and
- a preliminary list of EU lower priority substances ranked in order of priority (if lower priority nominations have been invited).

Ranking of substances within the higher and lower priority lists is independent. For substances prioritised on the basis of an approximate 4hLC$_{50}$ derived from a poor toxicological database, this stage includes screening to check that a more reliable 4hLC$_{50}$ based on more detailed

[7] For example, for the Validation Exercise we used approximate 4hLC$_{50}$ values from an HSE database supplemented with values from elsewhere as necessary. Details are given in the spreadsheet at Appendix 3. We note that the IUCLID database [Heirdorn et al., 1996] is another possible source of approximate 4hLC$_{50}$ data. However this needs to be used with caution as it has not been subjected to critical appraisal; we therefore chose to use data from schemes in which the toxicity data has been critical appraised.

[8] Where a query might entail sensitive information on details for a particular site, the technical support team would need to ask MAHB to handle the query.

analysis does not affect their priority status and in particular that substances do not fall out of scope.

F) Stakeholder Consultation
The preliminary higher and low priority lists are supplemented with any additional information of interest to stakeholders which has not been used in prioritisation[9]. Any precursor substances identified by Competent Authorities will also be listed as will any nominated substances which are out-of-scope for AETLs development and the 21 case study substances for which AETLs have already been developed.

Major EU stakeholders are then consulted on the preliminary higher and lower priority substance lists. Views sought will include whether any further substances should be included, and whether the substance rankings are appropriate. According to the judgement of the AETLs Selection Committee, the priority lists are modified as necessary.

G) Value for Money Considerations Give AETL Development List
The AETL Selection Committee decides how many priority substances go forward initially for further AETLs development. This is essentially a policy decision where the 'cut-off' to decide how far down the priority list to go will be informed by considerations such as value for money, and the resource which can be allocated by year. For example, all the higher priority substances might initially go forward for AETLs development; or only those with greatest rank, or all the higher priority substances together with the lower-priority substances of greatest rank.

The outcome of this stage will be:

- the initial list of substances for further AETLs development;
- a list of those higher priority substances which are not on the initial list of substances for further AETLs development;
- a list of those lower priority substances which are not on the initial list of substances for further AETLs development (if lower priority nominations have been invited);
- a list of any nominated substances which are out-of-scope for AETLs development; and
- a list of any precursor substances identified by Competent Authorities.

H) AETL Development with 4hLC_{50} Screening
AETLs are developed. This stage includes further screening (as done at Stage E) to check that a more reliable 4hLC_{50} based on more detailed analysis does not affect substances priority status and in particular that substances do not fall out of scope.

I) Keep AETL Development List Under Review
During AETLs development, the list of substances for which AETLs is being developed is kept under review by the AETLs Selection Committee so that the changing needs of stakeholders can be taken into account as necessary.

J) Member States Already Nominated Lower Priority Substances?
If prioritisation began with Member States nominating only their higher priority substances, the prioritisation process is repeated for their lower priority substances.

[9]The Critical Review Panel will advise on this information. So far as we understand, at this stage some members have suggested that it would be helpful to include the availability of various other thresholds including US 'IDLHs' [Alexeeff, 1989] and 'ERPGs' [Rusch, 1993]. This would be as background information and would not affect prioritisation.

The process described above gives a first EU list of substances for further AETLs development. Subsequent lists could be selected using the same approach and asking Member States for any modifications to their nominations. Additionally, individual Member States may choose to develop an AETL for adoption by the EU for any of their priority substances which are not included on the first EU list of substances for further AETLs development.

5.2 THE SIX PRIORITISATION CRITERIA

In this section we describe the six prioritisation criteria. There is one selection criterion (S1) and five ranking criteria (R1 to R5). As previously discussed, the ranking criteria are informed by considerations of off-site risk/hazard to the public. The criteria are summarised in figure 5.1 which corresponds to Stages E, F and G of the flowchart. As shown in the flowchart, the outcome of applying the criteria to substances nominated by Competent Authorities, together with consideration of EU policy issues, is a preliminary EU higher priority substance list and a lower priority substance list where the substances in each list are ranked in order of priority. Subject to stakeholder consultation, and value for money considerations, the EU first list of substances for AETLs development will be selected from these higher priority and lower priority lists.

5.2.1 Criterion S1: Select Substances In Scope

This criterion is to select substances that are in-scope. The scope being advised by the Critical Review Panel at this time was described in Chapter 3 and may be summarised as substances which are Toxic, Very Toxic, Named Carcinogens in the Seveso II Directive, Corrosive or Irritant. As described in Chapter 3, additional categories of substances may be considered as in-scope on the basis of expert judgment. The supporting information provided by the nominating Competent Authority will be one of the considerations informing this judgment.

5.2.2 Criterion R1: Rank Substances According to Link to Seveso II Sites or Equivalent For Corrosives and Irritants

This criterion is applied separately to: Toxics, Very Toxics and Seveso II Named Carcinogens; and to Irritants and Corrosives.

5.2.2.1 Toxics, Very Toxics and Seveso II Named Carcinogens

Substances which are Toxic, Very Toxic based on EU labelling criteria for dangerous substances or Named Carcinogens are assigned to the:

Preliminary EU Higher Priority List:	if they contribute significantly to the hazard/risk from top-tier sites; and
Preliminary EU Lower Priority List:	if they contribute to the hazard/risk from any Seveso II sites (top-tier and lower-tier).

This is done on the basis of the information supplied by the Competent Authorities at the nomination stage (Stage A in flowchart 5.1). Where appropriate, nominations will be checked (Stage D in flowchart 5.1).

The aim in ranking substances on the basis of the hazard/risk at Seveso II Directive top-tier sites is to take a pragmatic approach which will be acceptable and transparent across the EU. We have not given any suggested guidelines on what constitutes a significant contribution to off-site hazard/risk. In particular we consider that guidelines based on tonnages in excess of a specified fraction of the Qualifying Quantity would not be appropriate because the Qualifying Quantities were not set solely on the grounds of hazardous properties, rather policy considerations were also significant.

It should also be stressed that the off-site risk/hazard from a top-tier site is not necessarily greater than that from a lower-tier site. In addition to the way the Qualifying Quantities were set, for any given site, the population in the vicinity is an important factor in terms of the scale of the risk/hazard. Similarly, a top-tier site may hold less than the Qualifying Quantity at a particular time, while a lower-tier site may hold just less than the top-tier Qualifying Quantity. Therefore this criterion is a pragmatic one which we suggest as being fit for the purpose of prioritisation.

5.2.2.2 Irritants and Corrosives

Irritants and corrosives are assigned to either the preliminary higher priority or lower priority lists according to whether their potential to cause off-site harm is comparable to that for the nominated Toxic and Very Toxic substances in the higher priority or in the lower priority lists. This will be done by comparing the substance hazard measures: solids and fluids are compared separately. (See Chapter 6 for details.) If the nominating competent authority has opted to give an indicative priority and this does not accord with the assignment to the higher priority or lower priority list, the reason for the indicative priority will be queried at the nomination checking stage. We note that only 1 of the further 162 substances nominated during the Validation Exercise was a Corrosive or Irritant, it was nominated with an indicative lower priority.

5.2.3 Criterion R2: Give Higher Rank to Substances Nominated by More than One Member State

This criterion was chosen because developing AETLs for these substances will maximise their usefulness across the EU.

5.2.4 Criterion R3: Give Higher Rank to Substances According to their Potential to Cause Off-Site Harm Based on Physicochemical and Toxicological Hazardous Properties and Quantity

Chapter 6 gives technical details of the hazard measures used to rank substances according to their potential to cause off-site harm.

5.2.5 Criterion R4 (Optional): Give Higher Rank to Substances Linked to Multiple Seveso II Sites

This is an optional criterion which can be used as a 'tie-breaker' where substances have a similar rank based on the previous criteria. We envisage that little, if any, use will be made of this criterion. It might, for example, be helpful to use if a cut-off determined by financial considerations is being applied to the lists of priority substances to give a first EU list for AETLs development (Stage G in flowchart 5.1), where this cut-off falls in a group of otherwise similarly ranked substances. This criterion cannot be applied to Corrosive and Irritant substances.

We consider that the most pertinent information would be whether the substance dominates the off-site risk/hazard for a site. This would be for top-tier sites for substances on the higher priority list, and lower-tier sites for substances on the lower-priority list. However, this information was readily available for only one of the three Competent Authorities involved in the Validation Exercise. Other information related to numbers of sites was readily available for the other two Competent Authorities. So far as we understand, their information is related to the number of sites at which a substance is present at some level. Although we consider that the value of such information for ranking purposes is very limited it may, in the event that a 'tie-breaker' is needed, be of some use.

5.2.6 Criterion R5: Where Appropriate Modify Rank According to National-Level Issues for Individual Competent Authorities

The final criterion is to allow consideration of any additional national-level issues that might be proposed by individual Competent Authorities[10]. Any such additional issues would need to be considered on a case-by-case basis by the Selection Committee. An example of a national level issue, there may be special concerns regarding substances which do not meet Criterion S1 but have the potential to cause neurotoxicity.

5.3 COMMENTS ON THE PRIORITISATION METHODOLOGY AND CRITERIA

In the concluding section of the chapter we comment on the role of expert judgment in applying the criteria, the independence of the criteria from the availability of toxicological data or other substance thresholds, the need to establish the relative importance which will be accorded to the ranking by number of Member State nominations and by potential for off-site harm, and the need for further stakeholder consultation in the event that a further AETLs program is agreed.

[10] For example, as part of the Validation Exercise, the UK nominated 121 substances which would be considered for the preliminary lower priority substance list and which are not already included in the 21 preliminary ACUTEX case study substances. Of these 121 substances, 6 were identified as being of particular importance to the UK for AETLs development.

5.3.1 The Role of Expert Judgment in Applying the Criteria

A degree of expert judgment will be needed in applying the criteria. For instance, during the Validation Exercise, some groups of substances were nominated[11]. Here, judgment would be needed as to how to deal with substances in a nominated group taking into account why the nomination was originally made in this way. Additionally, consideration could be given to the grouping for AETL development of very closely related substances that have been nominated individually.

5.3.2 Prioritisation is Independent of the Availability of Toxicological Data

We note that prioritisation is independent of the availability of toxicological data. Therefore it is possible that there will be EU priority substances for which it is not technically possible to develop AETLs because of the limitations of the toxicological data available[12]. Therefore, if an AETLs program goes ahead, the EU body charged with overseeing this may wish to consider whether such substances should be the subject of a toxicity testing program.

5.3.3 Prioritisation is Independent of the Existence of Other Thresholds

We note that prioritisation is independent of the existence of other thresholds which can be used in relation to emergency planning and land-use planning for chemical plant. The reason is that a further AETLs program would be dependent on AETLs being found to be the most appropriate thresholds in an EU context.

5.3.4 The Relative Importance for Ranking of Number of Nominations and Potential for Off-Site Harm

At this time, the relative importance in the ranking process of the number of Member State nominations and the potential for off-site harm for a substance has not been decided. This is a policy matter left for consideration by the Competent Authorities and the Critical Review Panel.

5.3.5 The Need for Further Stakeholder Consultation if a Further AETLs Program is Agreed

As already noted, the methodology will be reviewed in the event that a further AETLs program is agreed. For example, if the money initially available for an AETLs program would only cover higher priority substances, then initial Member State nominations might be invited for these substances alone. Equally, ranking of these higher priority substances may be unnecessary if the funding would cover AETLs development for all of them. Similarly, any changes to data availability would need to be taken into account. For instance, if information on potential release tonnages were in future available (for example, expressed as typical tonnages of concern for a substance) the methodology could be modified accordingly.

[11] For example, as part of the Validation Exercise, the UK identified ‘nickel compounds’ as a priority.

[12] The need to explore the limits of the AETL methodology with respect to data-poor substances at the stage of the AETL methodology development was taken into account in determining the criteria for selection of the 21 ACUTEX case study substances, see [Trainor et al., 2003].

6 TECHNICAL DETAILS ON HAZARD MEASURES FOR 'POTENTIAL TO CAUSE OFF-SITE HARM'

The prioritisation criteria R1 and R3 (see section 5.2 above) make use of hazard measures to rank substances according to their potential to cause off-site harm based on physicochemical and toxicological hazardous properties together with tonnage. They are summarised in table 6.1. We note that before proposing these criteria, we checked with MAHB that there are no existing EU hazard measures or ranking approaches in relation to the Seveso II Directive that could be used for prioritisation purposes.

Table 6.1: Summary of Hazard Measures:

		Substance Type		
		Toxic & Very Toxic Substances	Irritant and Corrosive Substances	Seveso II Named Carcinogens
Physical State at 20°C and Atmospheric Pressure	Fluids (Vapours or Liquids)	***- 20 te Plume Area (4hLC$_{50}$ footprint)*** with supplementary information on ***- 20 te Plume Downwind Extent*** & ***- Qualifying Quantity* Plume Area (4hLC$_{50}$ footprint)*** with supplementary information on ***-Qualifying Quantity* Plume Downwind Extent***	Same with potential release tonnage in place of Qualifying Quantity	Expert Judgment
	Solids	***-1/ 4hLC$_{50}$*** & ***- Qualifying Quantity*/4hLC$_{50}$***	Same with potential release tonnage in place of Qualifying Quantity	

* Qualifying Quantity for Toxic and Very Toxic Substances refers to the Top-tier Qualifying Quantity for substances assigned to the higher-priority substance list, and to the Lower-tier Qualifying Quantity for substances assigned to the lower-priority substance list.

In this chapter we begin with an overview of all the hazard measures. We then describe the hazard measures for fluids and solids in detail. This includes the need for a sensitivity analysis to be carried out once the models to be used have been agreed, and the possibility of using a parametrised hazard measure for fluids. Finally we stress the need for expert judgement in using the hazard measures.

6.1 OVERVIEW OF HAZARD MEASURES

6.1.1 Named Carcinogens

Substances that are Named Carcinogens[13] are ranked separately by expert judgment. One possibility is that it may be appropriate to consider Named Carcinogens as having a higher prioritisation rank than other substances. This is because of the high level of concern accorded to the Named Carcinogens at EU level as evidenced in their low qualifying quantities in the Seveso II Directive[14]. We do not consider them further.

6.1.2 Toxic, Very Toxic, Irritant and Corrosive Substances

For substances that are Toxic, Very Toxic, Irritant or Corrosive the hazard measures are based on substances' physicochemical and toxicological hazardous properties together with tonnage. These are estimated according to whether a substance is a solid or fluid. (Fluids are liquids or vapours). This refers to a substance's physical state at 20 ^{o}C and atmospheric pressure. Because vapours which cannot be stored as liquids are rare[15] we do not consider them further; they will be ranked on the basis of expert judgment. The hazard measures use an estimate of the $4hLC_{50}$ as an indication of relative toxicity. The reason for this was discussed in section 4.1.4 above. Substances that are in-scope on the basis of misclassification (see section 3.1.2) are handled on the basis of the classification used to decide that they are in scope.

The hazard measures rank solids and fluids separately; they do not allow solids and fluids to be ranked relative to one another. Rather this would need to be done by expert judgment. There are two reasons why we consider this is appropriate:

- The majority of substances under consideration are likely to be fluids[16].
- So far as we are aware, no EU-wide criteria exist which would provide a basis for this comparison. (Rather, within individual Member States a range of criteria based on, for example, dose, have been developed.)

For both solids and fluids there are two hazard measures. The first gives a rough indication of the relative hazard posed by substances independent of release quantities, while the second takes hypothetical release quantities into account. The latter uses the Seveso II Qualifying Quantities for Toxic and Very Toxic substances, and the potential off-site release tonnage as identified by the nominating Competent Authority for Irritant and Corrosive substances[17].

---

[13] The Named Carcinogens are thought to pose a risk of carcinogenicity following a single exposure, and are often termed 'one-shot carcinogens'. They are therefore acutely toxic.

[14] The qualifying quantities are 2 te for top-tier and 0.5 te for lower-tier sites compared to, for example, the upper tier and lower-tier qualifying quantities of 5 te and 20 te for Very Toxic substances.

[15] For example, only one such substances, fluorine, was among the 39 in-scope substances proposed by Competent Authorities which were used as a basis of the 21 ACUTEX case study substances [Trainor et al., 2003].

[16] For example, of the 39 substances proposed by Competent Authorities in their lists of '10 Substances of Interest' which were in-scope for the case study substances [Trainor, 2003], 34 (about 93%) are fluids.

[17] For Toxics and Very Toxics the potential off-site release tonnage could be used if a Competent Authority decides to provide this information. For example, a Competent Authority might wish to do this at the Stakeholder Consultation Stage of the prioritisation process (Stage F in flowchart 5.1) if they

6.2 HAZARD MEASURE FOR FLUIDS (LIQUIDS AND VAPOURS)

The two hazard measures give the area in km^2 which would be covered by a plume for the following hypothetical catastrophic release quantities:

- a 20 te reference quantity; and
- the Seveso II Qualifying Quantity for Toxics and Very Toxics, and the potential off-site release tonnage for Irritants and Corrosives.

The hazard measures would be given together with supplementary information on the plume downwind extent in km. This is for the plume $4hLC_{50}$ footprint.

We suggest using F2 weather conditions as a realistic 'worst case' scenario[18]. Similarly, where it is common practice to store a substance in more than one way, we suggest taking the worst-case storage conditions[19]. The plume area can be calculated using an appropriate gas dispersion code, taking due account of whether the released substance would give rise to a buoyant, passive or dense plume. We anticipate that under catastrophic failure conditions most if not all of the substances of interest will give rise to dense plumes which become passive as air is entrained. A description of consequence modelling for toxic releases is given in, for example, [CPD, 1997] and [Britter & McQuaid, 1988].

The hazard measure using the reference quantity will give a rough indication of the relative hazard posed by substances independent of quantity. A 20 te reference quantity is used because it is typical of the volumes of many substances stored at user (as opposed to manufacturing) sites. It is a typical quantity because the standard quantity stored in road/rail tankers is of the order of 20 tonnes[20]. Of course, many substances are held (and transported) in much smaller quantities. For example, for the highly volatile phosgene (carbonyl dichloride), this is reflected in the relatively low Qualifying Quantities it is given as a Named Substance in the Seveso II Directive: 0.3 te and 0.75 te for top-tier and lower-tier sites respectively.

For Toxic and Very Toxic substances, the hazard measure using the Seveso II Directive Qualifying Quantity will give a rough indication of the relative hazard posed by substances taking into account these quantities. For Toxic and Very Toxic substances assigned to the higher priority list, this is the top-tier (Article 9) Qualifying Quantity, while for those assigned to the lower priority list this is the lower-tier Qualifying Quantity. Of course, the actual quantity released on a particular Seveso II site may be either larger than the Qualifying Quantity (if the amount stored is higher), or lower (according to the proportion of the total site inventory released, whether a site has less than the maximum possible inventory stored, whether the

---

consider that the rank of a substance in the priority lists should be increased because the potential release tonnage for a specific site is far in excess of the Qualifying Quantity.

[18] [Lines and Deaves, 1997] discuss worst-case conditions in terms of hazard range or risk and note that F2 weather conditions are often used. 'F2' refers to stability class and wind speed, for a description of weather classes see [CDP, 1999].

[19] For example, ammonia is commonly held in either refrigerated, semi-refrigerated, or ambient-temperature pressured storage. The worst case would be ambient-temperature storage as this would give rise to the largest quantity of toxic vapour produced on catastrophic failure.

[20] The quantity of a dangerous substance which may be transported are set by UN Regulations on the Transport of Dangerous Goods. Broadly, substances are in 9 classes (flammable, gases, explosives, oxidising, toxic, radioactive etc.) according to which they fall into one of 3 classes determining maximum transport size. Road/rail tankers are the largest size. For details see [UN, 2001].

Qualifying Quantity refers to the sum of a number of generic Toxic or Very Toxic substances[21], etc.).

For Corrosive and Irritant substances, the hazard measure using the potential off-site release tonnage will allow a substances to be assigned to the preliminary higher priority or lower priority list according to how the hazard measure compares with that for nominated Toxic and Very Toxic substances. Similarly, the results will allow Corrosive and Irritant substances to be ranked within these two lists.

6.3 DISCUSSION OF HAZARD MEASURES FOR FLUIDS

6.3.1 The Hazard Measures Are for Ranking Purposes Only

Firstly we stress that the hazard measures are solely for the purposes of *ranking* substances. Because the measures are based on the plume $4hLC_{50}$[22] footprint, the *absolute* values for the plume areas and extent are very large and are not intended to convey any meaning in relation to absolute hazard or risk. On the contrary, people on the perimeter of the $4hLC_{50}$ footprint certainly would not be exposed for a 4 hour period. Risk or hazard based studies used to inform land-use planning or emergency planning are generally based on plume footprints for a specified dose rather than concentration. (Dose takes into account both the duration of exposure and the concentration and is therefore directly linked to the likelihood of harm. Considering concentration independent of duration is not.) We consider that using concentration rather than dose is suitable for the purposes of substance ranking and that, in this context, has several advantages:

- $4h\text{-}LC_{50}$ is a widely recognised toxicity 'benchmark' value for toxicologists;
- there is no one definition of dose in use across the EU to inform risk/hazard studies in relation to Seveso II sites;
- estimation of the dose received within a plume requires assumptions about the exposure time which includes complex considerations of the plume passage time and possible escape behaviour of people[23].

Similarly, we consider that the specific gas dispersion and pool formation and evaporation models used is not an issue provided that they are fit-for-purpose and supported by a peer-reviewed publication. (The use of consistent models and assumptions for the different substances is, of course, essential.) Again, this is because the outcome is to be used for *ranking* purposes, rather than to give absolute plume areas and extent. In other words, although different models will give different absolute values for plume areas and extent, there should be reasonable agreement on the rank of substances according to plume area.

The work of the EU Model Evaluation Group which included gas dispersion is described in [Petersen, 1999]. Also pertinent is the outcome of the European Benchmark Exercise which considered a reference ammonia plant and found that the choice and use of models contribute to differences in absolute risk estimations [Amendola, 1992], and the work of the more recent EU

[21] The Qualifying Quantity applies either to the amount of a Named Substance, or to the total amount of all the substances within one of the generic categories.

[22] Note that when there are LC_{50} values available for several laboratory species the hazard measure will normally be based on the value for the more sensitive species, unless there is evidence to indicate that one of the other species is more relevant to humans.

[23] Additionally, in practice, assessment methods distinguish between indoor and outdoor dose.

'Assurance' project which also benchmarked risk estimates for a reference ammonia plant and considered the effect of variation in the assumptions and modelling approaches of the project partners [Markert et al., 2001].

6.3.2 Need for a Sensitivity Analysis to Indicate Accuracy of Rank

To use the hazard measures for ranking purposes, it would be desirable to have an indication of their accuracy. In other words, what percentage difference in plume area is needed for substances to have a different rank? We suggest that in order to address this, a sensitivity study would need to be carried out. For example, this could consider the effect on plume area of a 10% variation in $4hLC_{50}$, etc. This would need to be done for substances with a range of physical state, toxicity and dispersion characteristics. We have included this in Stage 0 of flowchart 5.1 where it would be done after selection of the models.

6.3.3 Possible Use of Hazard Measure for Fluids Based on Parametrization of Substance Properties

It may be possible to replace the hazard measure with:

- a parametrization based on substance properties in place of the plume area for the reference quantity; and
- the same parametrization taken together with the Qualifying Quantity, in place of the plume area for the Qualifying Quantity.

Here the Qualifying Quantity applies to Toxic and Very Toxic substances, while the potential off-site release tonnage applies instead for Corrosive and Irritant substances.

For example, Canadian regulatory work [Lacoursiere, 2002] in support of defining threshold quantities in respect of potential releases of toxic substances from chemical plant uses a ranking factor based on substance inherent properties. See Appendix 6 for details. Similarly, an indicative ranking measure developed at HSE for the hazardous potential of liquids is the ratio:

$$VP/\ LC_{50}\ (\text{inhalation})$$

where VP is the vapour pressure at ambient temperature. (For further details see [Trainor et al., 2003].) So far as we are aware from MAHB, no EU measure has been developed specifically for a Seveso II context.

Such parametrizations are based on toxicity, together with a much simplified description of dispersion. Essentially, for dense releases, plume extent to a given concentration correlates with the release volume of gas/vapour [Britter & McQuaid, 1988]. Many pressure liquefied gases will, in the worst case, vaporise completely on loss of containment due to jet entrainment. Less volatile substances will give rise to a smaller release volume per release mass because much less of the substance will evaporate. Therefore, for less volatile substances the plume extent to a given concentration will be smaller than for the highly volatile substances.

We suggest that the full hazard measures (i.e. plume rank with supporting information on downwind extent) should be used for the substances assigned to the preliminary higher priority substance list (the top-tier or equivalent substances). The results could then be used to test

whether a parametrization would be suitable. If so, the parametrization could be used for the substances assigned to the preliminary lower priority substances list *provided* it gives a significant saving in cost. We have included this in the description of Stage C of flowchart 5.1.

6.3.3.1 Example of Hazard Measures for 4 Fluid Substances

Table 6.2 illustrates the hazard measures for 4 of the substances that were nominated by Competent Authorities in their lists of '10 Substances of Interest' (see Section 1.2):

- Chlorine, ammonia and sulphur dioxide are Toxic substances.
- Monomethylamine is in scope as a misclassified Toxic substance.

Appendix 7 gives details of the calculations and models used to generate the hazard measures.

Additionally, in the substances spreadsheet in Appendix 3, we give a very crude demonstration of the effect of Qualifying Quantity on rank for a larger number of substances. The spreadsheet gives the indicative hazard measure

$$VP/\ 4hLC_{50}$$

and shows how the substances are ranked according to this indicative measure. It also shows how the substances are ranked if the indicative hazard measure

$$\text{Top-tier Quantifying Quantity} \times VP/\ 4hLC_{50}$$

is used instead.

In both cases, 1 is the highest rank or greatest hazard. We stress that these indicative hazard measures are used for the purpose of this demonstration only: they are not intended to replace the hazard measures.

It can be seen that the rank of the substances changes. For example, the rank for phosgene reduces from 1 to 16 when Qualifying Quantity is taken into account, while the rank for sulphur dioxide increases from 15 to 7 when Qualifying Quantity is taken into account.

Table 6.2: Illustration of Hazard Measures for Four Fluids

Substance with CAS Number	**Physical State**	**Approx. $4hLC_{50}$**		**Hypothetical Catastrophic Release of 20 te (F2 Weather Conditions)**					**Seveso II Qualifying Quantity**	**Hypothetical Catastrophic Release of Qualifying Quantity (F2 Weather Conditions)**				
		(mg/l)	**(ppm)**	**Plume Half Width (km)**	**Plume Down-wind Extent (km)**	**Plume Up-wind Extent (km)**	**Approx. Plume Area (km^2)**	**Rank by Area 1= Highest**	**(te)**	**Plume Half Width (km)**	**Plume Down-wind Extent (km)**	**Plume Up-wind Extent (km)**	**Approx. Plume Area (km^2)**	**Rank by Area 1= Highest**
Ammonia 7664-41-7	G	1.47	$2.07x10^{3}$	$4.18x10^{-1}$	1.47	$1.38x10^{-1}$	1.06	2	200 Seveso II Generic Toxic	1.04	3.69	$3.92x10^{-1}$	6.64	2
Chlorine 7782-50-5	G	$1.33x10^{-1}$	$4.49x10^{1}$	$7.44x10^{-1}$	$1.77x10^{1}$	$9.80x10^{-2}$	$2.11x10^{1}$	1	25 Seveso II Named Substance	$8.42x10^{-1}$	$2.04x10^{1}$	$1.08x10^{-1}$	$2.71x10^{1}$	1
Sulphur Dioxide 7446-09-5	G	1.49	$5.57x10^{2}$	$3.84x10^{-1}$	1.75	$9.90x10^{-2}$	1.12	2	200 Seveso II Generic Toxic	$9.58x10^{-1}$	4.30	$2.89x10^{-1}$	6.91	2
Mono-methyl-amine 74-89-5	G	1.20	$9.47x10^{2}$	$3.45x10^{-1}$	1.63	$1.24x10^{-1}$	$9.51x10^{-1}$	2	200 Seveso II Generic Toxic	$8.56x10^{-1}$	4.28	$4.00x10^{-1}$	6.30	2

6.4 HAZARD MEASURE FOR SOLIDS

For solids, we again give two hazard measures.

The first hazard measure is to prioritise according to $1/4hLC_{50}$: that is to say the lower the $4hLC_{50}$ the greater the toxicity. This is based on the potential for solids to be dispersed off-site in fires (for example warehouse fires). Not all of a solid will be dispersed in a fire plume, and some of what is dispersed will be carried sufficiently far away that it will not pose a risk. Therefore toxicity is a very crude measure of hazard[24]. It is not intended to be a definitive scientific assessment.

The second measure is to prioritise according to increasing:

Qualifying Quantity / $4hLC_{50}$	for Toxics and Very Toxics, or
Potential Release Tonnage/$4hLC_{50}$	for Irritants and Corrosives.

For Toxics and Very Toxics this is to give a rough indication of the relative hazard posed by substances taking into account the different Qualifying Quantities in the Seveso II Directive. Essentially, this takes account of the fact that the quantity of a Toxic substance held at a site may be much greater than for a Very Toxic substance because the Qualifying Quantity is greater. For substances assigned to the preliminary higher priority list, this is the top-tier (Article 9) Qualifying Quantity, while for substances assigned to the preliminary lower priority list, this is the lower-tier Qualifying Quantity. As described above for fluids, the actual release quantity may be either greater or less than the Qualifying Quantity.

As described above for fluids, for Irritants and Corrosives, the potential off-site release quantity as identified by the nominating Competent Authority is used to allow these substances to be nominated to the preliminary higher or lower priority lists, and to allow them to be ranked within those lists.

6.5 DISCUSSION OF HAZARD MEASURES FOR SOLIDS

6.5.1 Why a More Detailed Approach is not Appropriate for Solids

We also considered the possibility of using a more detailed hazard measure in line with those for fluids.

Aspects of modelling warehouse fires are described in [Atkinson & Hill, 1999], [McBride & Atkinson, 2004] and [Maddison et al., 1996]. Within HSL, for example, warehouse fire modelling is carried out on behalf of HSE using the in-house FIREPEST model [Maddison et al., 1996]. Factors influencing the potential for harm of a substance include:

1.) the flammability and quantity of the substances it is stored with;
2.) the relative height at which the substance is stored (because of dispersal effects);

[24] We are grateful to Mr R. Rowlands, a Major Hazards specialist inspector at HSE, for suggesting this hazard measure to us.

3.) the flammability and size of packaging[25];
4.) the structure of the warehouse[26]; and
5.) the substance's own flammability and particle size (whether a solid is in the form of granules or particulates affects both entrainment into a fire plume and deposition from the plume).

There is considerable dependence on factors that are unrelated to a substance's inherent hazardous properties. Therefore, in our view, use of a more detailed hazard measure would not be appropriate.

6.5.2 Example of Hazard Measures for Solids

The spreadsheet at Appendix 3 shows how 5 solids are ranked according to these two measures. These are the 5 solids that were among the substances which formed the basis for selection of the 21 ACUTEX case-study substances (see section 1.2). (Solids formed approximately 13% of the of 39 substances nominated by Competent Authorities which were in-scope for the ACUTEX case studies.)

Additionally, consideration can be given to whether the potential for release during manufacturing (in addition to release during storage) is also significant. This would need to be done by expert judgment.

6.6 NEED FOR EXPERT JUDGEMENT IN USING THE HAZARD MEASURES FOR FLUIDS AND SOLIDS

We stress that expert judgement will be required when using the hazard measures. This includes taking into account not just the uncertainties in the modelling, but also the relevance of the Qualifying Quantity taking into account likely maximum release quantities depending on practice at manufacturing, storage and user sites.

[25] The higher the mass loss rate from a package is, the lower the efficiency of dispersion is. Therefore, in general there will be more dispersion from small packaged powders (approximately 1 to 25 kg) than large ones.

[26] In particular, if a warehouse roof remains intact then dispersion is much reduced, especially for larger particulates (greater than 50 microns) for which re-deposition within the warehouse would be significant.

7 INFORMATION RECEIVED FROM THE 3 COMPETENT AUTHORITIES AS PART OF THE VALIDATION EXERCISE

In this chapter we describe the information received from the UK, French and Italian Competent Authorities during the Validation Exercise and its implications. Particularly important considerations during the Validation Exercise were:

- the number of priority substances because this determines the degree of complexity needed in the prioritisation methodology;
- the degree of consensus in the priority substances, since if the consensus is high, the task of prioritisation is simplified;
- what information is readily available at Competent Authority level; and
- any national-level prioritisation issues.

We begin with the number of priority substances proposed by the three Competent Authorities involved in the Validation Exercise, and their significance. We then discuss the other prioritisation issues raised during the Validation exercise. We conclude with a section describing the basis used by each Competent Authority for their nominations. We suggest that this concluding section could be excluded from the publicly available final report.

7.1 NUMBER OF SUBSTANCES PROPOSED BY THE FRENCH, ITALIAN AND UK COMPETENT AUTHORITIES AND THEIR SIGNIFICANCE

7.1.1 Proportion of EU Seveso II Sites in the Member States Involved in the Validation Exercise

Table 7.1 shows the number of Seveso II sites in France, Italy and the UK as an *approximate* percentage of the total in the 15 EU Member States based on 2001 and 2002 data. It can be seen that they have approximately 50% of all EU Seveso II sites for the 15 Member States. Additionally, they account for between approximately 40% and 50% of Seveso II sites in the 25 EU Member States as of 1 May 2004[27]. Therefore, we consider that the outcome of the Validation Exercise can be used to give a reasonable indication of the position for the EU as a whole in terms of number and degree of consensus in proposed substances and the implications for further AETLs prioritisation.

[27] Information on percentage numbers of sites for the 15 Members Sites in 2001/2002, and for all 25 current Member Sites is from MAHB. Because data from some Member States is currently being clarified or not yet held the percentages quoted are *approximate* only.

Table 7.1: Number of Seveso II Sites as a Percentage of the Total for the 15 EU Member States and Numbers of In-Scope Priority Substances Proposed During the Validation Exercise.

Competent Authority	Seveso II Sites as a % of the Total for the 15 EU Member States, 2001/02	Number of Proposed Substances			Number of Proposed Substances NOT Included in the 21 Preliminary Case Study Substances		
		High Priority	Lower Priority	Total	High Priority	Lower Priority	Total
Italy	16.5 %	23	12	36	12	9	21
France	16.0 %	13	19	32	3	14	17
UK	19.2 %	25	129	154	12	121	133
Total	51.7 %	34	145	162	19	134	141
Total Proposed by at Least 2 of the 3 Competent Authorities	-	18	14	42	7	10	26

It is interesting to note that of the 19 High Priority substances which are not included in the 21 case studies, 6 neither have AEGLs nor are not currently on the AEGL program. Similarly, of the 132 lower priority substances not among the case studies, 106 neither have AEGLs nor are not currently on the AEGL program.

7.1.2 Number of Proposed Substances

Table 7.1 also gives the number of priority substances proposed by the French, Italian and UK Competent Authorities during the Validation Exercise. The table shows only those substances which are in the scope being advised by the ACUTEX Critical Review Panel. One out-of-scope substance was also proposed: we have not been given any information on why this is considered to be relevant for AETLs development.

7.1.3 Precursor Substances

All three Competent Authorities included precursor substances with their nominated priority substances. A precursor substance is one which is not to be considered for AETLs development, but which is relevant because a proposed priority substance is one of its reaction products. In other words, consideration of the potential for release of these precursors is an important consideration in identifying the priority substances.

7.1.4 Implications of Numbers of Proposed Substances for Further AETLs Development

The three Competent Authorities proposed 19 higher priority substances that are not already included in the 21 preliminary ACUTEX case study substances. They are the ‘new’ higher

priority candidates for AETLs development. Of these 19 new substances, 7 (37%) were proposed by at least 2 of the 3 Competent Authorities. The Competent Authorities also proposed 134 new lower priority candidates for AETLs development of which 10 (7%) were proposed by at least 2 of the 3 Competent Authorities. We note that, as can be seen from table 7.1, the numbers of priority substances differ significantly for the three Competent Authorities. So far as we are aware, these differences are related in part to the differences in availability of appropriate information within the Competent Authorities.

These results were discussed at the Validation Workshop. Overall, we consider that they may be taken as indicating that the total number of new EU higher priority candidates for AETLs development is unlikely to be much in excess of 50. The implications of this were discussed at the Validation Workshop. While value for money considerations cannot be pre-judged, it was suggested that this raises the possibility that all the EU higher priority substances could be included in a first EU list of substances for AETLs development in the event of a further program of AETLs development. If this is the case, then ranking of the higher priority substances may be unnecessary.

Additionally, we consider that the total number of priority substances indicates that the straightforward AETL prioritisation methodology we have developed is appropriate for the likely number of EU-wide priority substances.

7.2 PRIORITISATION ISSUES RAISED DURING THE VALIDATION EXERCISE

Here we discuss the outcome of the consideration of EU and national-level issues for prioritisation, and the availability of information on numbers of sites for nominated substances.

7.2.1 EU-Level Prioritisation Issues

A number of EU-level prioritisation issues were raised as a result of the information provided by the 3 competent authorities. These were discussed at the workshop and have all been taken into account in the updated scope of substances and methodology described in this report.

7.2.2 Additional National-Level Prioritisation Issues

No additional national-level prioritisation issues were identified by the French and Italian Competent Authorities. One issue was identified by the UK Competent Authority (see details below). Within the prioritisation methodology, this issue could be considered under prioritisation criterion R5 described in section 5.2.6 above.

7.2.3 Information Available from the 3 Competent Authorities on Numbers of Sites

As discussed in section 5.2.5, an optional prioritisation criterion (R4) is to rank substances according to the number of Seveso II sites at which they dominate the off-site risk/hazard. This is for top-tier sites for higher priority substances, and lower-tier sites for lower priority

substances. This criterion could be used if necessary as a 'tie-breaker' where a number of substances otherwise have the same rank.

This prioritisation criterion is optional because during the Validation Exercise it was found that the information would be readily available to only one of the three Competent Authorities, the UK, where it is being considered for other purposes. Therefore it was considered unlikely that it would be readily available for many Member States. For the higher priority UK substances, the number of top-sites for each substance varies between 1 and 35. This UK information was considered at the Validation Workshop and found to be suitable for prioritisation purposes.

For France and Italy, other information related to numbers of sites is available. We have not received details of how this information was derived, but, so far as we understand, it is related to the number of sites at which a substance is present at some level. Although we consider that the value of such information for ranking purposes is very limited it may, in the event that a 'tie-breaker' is needed, be of some use where full details of the derivation method used are supplied by the Competent Authorities.

7.3 BASIS OF PRIORITY SUBSTANCES PROPOSED BY ITALY, FRANCE AND THE UK

7.3.1 Basis of Priority Substances Proposed by Ministere de L'Ecologie et du Developpement Durable for the French Competent Authority

The French priority substances are based on a number of considerations including: a substance's acute toxicity; whether there is a specific French classification for installations using the substance; and the priorities of the French Inspection.

No national level issues for prioritisation were identified and the French substances were not ranked within their higher and lower priority lists.

7.3.2 Basis of Priority Substances Proposed by ISPESL for the Italian Competent Authority[28]

The Italian priority substances are based on information in an existing database on Seveso II sites which includes information for sites on which substances which can potentially be released. The database is maintained by the Ministry of the Environment. Risk/hazard was the basis of prioritisation.

No national level issues for prioritisation were identified and the Italian substances were not ranked within their higher and lower priority lists.

[28] ISPESL is part of the Italian Competent Authority which also includes the Ministry of the Environment.

7.3.3 Basis of Priority Substances Proposed by HSE for the UK Competent Authority[29]

HSE's final priorities for AETLs will depend on the outcome of ACUTEX. The information on priority substances given below has been provided by HSE solely to inform the development of the prioritisation methodology.

HSE's proposed priority substances, and the criteria used to select them, were the subject of a UK stakeholder consultation exercise[30]. The list of 154 priority substances was taken directly from the HSE list at http:/www.hse.gov.uk/hid/haztox.htm. This is a publicly available list which gives HSE's land-use planning toxicity threshold (the SLOD/SLOT). The list was started in 1990 as a compilation of toxicological data used by HSE:

a) to assess safety reports for Seveso I and Seveso II sites; and
b) to give advice on land-use planning in the vicinity of Seveso sites.

In other words, the 154 priority substances are all the substances which HSE has 'screened' for their potential to pose off-site risks when giving land-use planning advice or assessing safety reports. Producing the list of UK priority substances was very straightforward because it was taken directly from this existing list.

7.3.3.1 UK Higher Priority Substances

Out of the 154 substances, HSE identified 25 high priority substances. They are the substances which are considered to be most significant in terms of the potential for off-site harm from UK top-tier sites. This takes into account issues such as inherent hazardous properties, potential release tonnage and storage type. The substances were identified by specialist Major Hazards inspectors based on quantitative studies of top-tier sites HSE had previously carried out for other purposes.

7.3.3.2 UK Lower Priority Substances

The remaining 129 substances are the UK lower priority substances. Of these 6 have a higher rank for the UK while the remainder have a lower rank for the UK.

The 6 substances with a higher UK rank are used in the UK as "exemplar" substances; they are listed in table 7.2. The exemplars are "worst case" substances in terms of their inherent properties within the coverage of classification given in this table. This is a national-level issue for prioritisation.

[29] The UK Competent Authority comprises HSE, the Environment Agency and the Scottish Environmental Protection Agency. HSE leads on aspects of the Seveso II Directive which relate to harm to people.

[30] Major UK stakeholders were consulted through the Major Hazard's Subgroup of the Health and Safety Commission's Advisory Committee on Dangerous Substances (MHSC/ACDS), and through the Chemical and Pipeline Emergency Planning Liaison Group (CAP-EPLG).

Table 7.2: The 6 UK 'Exemplar' Substances

Substance			Coverage of classification
Name	Formula	CAS No.	
Methyl Chloroformate	$C_2H_3ClO_2$	79-22-1	***Very Toxic*[31] *fluid*** worst case
Methyl Iodide	CH_3I	74-88-4	***Toxic fluid*** high volatility range, worst case
Propionitrile	C_3H_5N	107-12-0	***Toxic fluid*** medium volatility range, worst case
Ethylene Dibromide	$C_2H_4Br_2$	106-93-4	***Toxic fluid*** low volatility range, worst case
Paraquat Dichloride	$C_{12}H_{14}N_2Cl_2$	1910-42-5	***Very Toxic Solid*** worst case
Lindane	$C_6H_6C_{16}$	58-89-9	***Toxic Solid*** worst case

[31] Note: Methyl Chloroformate is currently misclassified in Annex 1 of the Dangerous Substances Directive as Toxic rather than Very Toxic. Reclassification as Very Toxic is expected by way of the next (29th) 'Adaptation to Technical Progress'.

8 TECHNICAL SUPPORT NEEDED FOR SUBSTANCE PRIORITISATION

The Technical Support Team would need to liaise closely with the AETL Selection Committee and with toxicologists developing the thresholds, particularly on the approximate 4hLC_{50} information. We recommend that technical support for substance prioritisation should include:

1.) Hazard information on proposed substances as described above in chapter 6. This requires the Technical Support Team to have in depth experience of:
   - gas dispersion modelling in terms of model development, application and use, and understanding of model limitations and uncertainties; and
   - making expert judgements on release scenarios and source term modelling.

2.) Provision of support on issues related to hazard information and its significance, as necessary. This would require familiarity with issues such as likely industrial use in storage, handling and quantities for common substances.

3.) A database to hold the information on substances proposed by Member States in relation to prioritisation criteria. This is to allow efficient manipulation and presentation of the information. Additionally, it allows flexibility for adapting the prioritisation methodology to future needs, for example arising from any broadening to the context in which AETLs are developed such as the inclusion of dangerous goods transportation.

4.) A website which can be accessed by Competent Authorities and other stakeholders using a password. This would initially display the substance nominated by each Competent Authority in order to facilitate nominations and nomination checking (for Stages A and D of prioritisation as given in flowchart 5.1). It would then display details of the prioritisation information used for each substance (for Stages E, F, G and I of prioritisation as given in flowchart 5.1). This would aid the transparency of the prioritisation process.

5.) Additionally, familiarity of the Technical Support Team with a wide range of Seveso II safety reports would be an advantage.

For example, HSL would be well placed to provide this support.

We note that consideration of the composition of the AETL Selection Committee is outside our remit. Rather, it would need to be addressed by the Critical Review Panel.

9 THE PRIORITISATION METHODOLOGY IN RELATION TO THE IDENTIFIED REQUIREMENTS

In section 2.3 we listed the 6 requirements that must be met by the prioritisation methodology for possible further AETLs development. These requirements have underpinned the work described in this report as summarised below.

The most important factor in meeting requirements 1 to 3 has been the overall approach we have adopted in developing the methodology. This approach was described in section 2.1. It may be summarised as stakeholder consultation at each stage of the development, and the involvement of three Competent Authorities in the Validation Exercise. Additionally, we aimed to develop criteria that are acceptable and transparent to EU major stakeholders by basing them on the Seveso II Directive taking into account commonalities in implementing the directive across EU Member States. This was described in Chapter 4.

We have aimed to meet requirement 4 on flexibility by proposing, in Chapter 8, the use of a substance database which can be extended as appropriate to take into account changing future needs.

In regard to requirement 5, we concluded that it is not practicable to base the methodology on existing methodologies, criteria and information. As described in Chapter 4, we have explored and rejected the possibility of basing the prioritisation on existing information because appropriate information does not exist. Additionally, as noted in Chapter 6, we checked with MAHB that there are no existing EU hazard measures or ranking approaches in relation to the Seveso II Directive that could be used for prioritisation purposes.

Finally, in regard to requirement 6, the important considerations in ensuring that the methodology is of a level of detail appropriate to the task, were again the use of stakeholder consultation, together with the information from the Validation Exercise, in particular the information indicating how many substances are likely to need to be prioritised.

10 REFERENCES

ACGIH, American Conference for Governmental Industrial Hygienists, Inc. (1986) *Documentation of the Threshold Limit Values and Biological Exposure Indices,* 5th Edition, ACGIH, Cinnnati, OH.

Alexeeff G.V., Lipsett M.J., and Kizer K.W. (1989) *Problems Associated with the Use of Immediately Dangerous to Life and Health (IDLH) Values for Estimating the Hazard of Accidental Chemical Releases,* Am. Ind. Hyg. Assoc. J. **50**(11): 598-605.

Alexeeff G., Lewis D. and Lipsett M. (1991) *Use of Toxicity Information in Risk Assessment for Accidental Releases of Toxic Gases,* J. Haz. Mat. **29**: 387-403.

Amendola A. (1992) *Uncertainties in Chemical Risk Assessment: Results of a European Benchmark Exercise,* J. Haz. Mat. **29:** 347-273.

Atkinson G. and Hill D.N. (1999) *Plume Seeding During Fires at Chemical Warehouses,* HSL Report FS/99/05, HSE Information Centre, Broad Lane, Sheffield S3 7ZL, UK.

Britter, R.E. and McQuaid, J. (1988) *Workbook on the Dispersion of Dense Gases,* HSE Contract Research Report No. 17/1988, HSE Information Centre, Broad Lane, Sheffield S3 7ZL, UK.

Cassidy K. and. Amendola A. (eds.) (1999) *Seveso II Special Edition,* J. Haz. Mat. **65** Nos.1-2.

Christou M.D., Amendola A. and Smeder M. (1999) *The Control of Major Accident Hazards: The Land-Use Planning Issue,* J. Haz. Mat. **65:** 151-178.

CPD, Committee for the Prevention of Disasters, Director-General for Social Affairs and Employment, Netherlands (1997) *Methods for the Calculation of Physical Effects,* Report CPR 14E, Sdu Uitgevers, The Hague, The Netherlands.

CPD, Committee for the Prevention of Disasters, Director General for Social Affairs and Employment, Netherlands (1999) *Guidelines for Quantitative Risk Assessment: Purple Book,* Report CPR 18E, Sdu Uitgevers, The Hague, The Netherlands.

Craig D.K., Davis J.S., Hansen D.J., Petrocchi A.J., Powell T.J. and Tuccinardi T.E. (2000) *Derivation of Temporary Emergency Exposure Limits,* J. Appl. Toxicol. **20**: 11-20.

Davis G.A., Swanson M. and Jones S., (1994) *Comparative Evaluation of Chemical Ranking and Scoring Methodologies,* EPA Order No. 3N-3545-NAEX, University of Tennessee Center for Clear Products and Clean Technologies, Knoxville, Tennessee.

ECETOC, European Chemical Industry, Ecology and Toxicology Centre (1991) *Emergency Indices for Industrial Chemicals,* Technical Report No. 43, ECETOC, Brussels.

EPA, Environmental Protection Agency (1997) *EPA Notice of Acute Exposure Guideline Levels,* Chemical Regulation Reporter **21**(31): 880-893.

EPA, Environmental Protection Agency (2001) *Overview of the Acute Exposure Guideline Levels (AEGL) Program: May 2001,* Washington (US): EPA. (Paper presented at the *Workshop*

on Acute Exposure Guideline Levels (AEGLs), 28-30 May 2001, Major Accident Hazards Bureau, Joint Research Centre, European Commission, Ispra, Italy.)

EPA, Environmental Protection Agency (2002) *Second List of Priority Chemicals for Guideline Development US Federal Register,* May 31 2001, **67**(105): 38106.

European Communities. Commission (1993) *Council Directive (EEC) 793/93 of 23 March 1993 on the Evaluation and Control of the Risks of Existing Substances,* O.J. European Communities 5.4.93, L 84: 1-8.

European Communities. Commission (1997) *Council Directive 96/82/EC of 9 December 1996 on the Control of Major Accident Hazards Involving Dangerous Substances*, O.J. European Communities 14.1.1997, L 10: 13-33.

European Commission (1999) *Study on the Prioritisation of Substances Dangerous to the Aquatic Environment,* Office for Official Publications of the European Communities, Luxembourg.

European Communities. Commission (2001) *White Paper on Risk Governance,* Series COM(2001)428 Final, Brussels.

European Communities. Commission (2002) *Report on the Application in the Member States of Directive 82/501/EEC*. O.J. European Communities 31.1.2002, C 28: 1-48.

European Communities. Commission (2003) *Directive 2003/105/EC of the European Parliament and of the Council of 16 December 2003 Amending Council Directive 96/82/EC on the Control of Major-Accident Hazards Involving Dangerous Substances*, O.J. European Union 31.12.2003, L 345: 97-105.

Fairhurst S. and Turner R.M. (1993) *Toxicological Assessments in Relation to Major Hazards*, J.Haz.Mat. **33:** 215-227.

Franks A.P., Harper P.J. and Bilio M. (1996) *The Relationship Between Risk of Death and Risk of Dangerous Dose for Toxic Substances,* J. Haz. Mat. **51:** 11-34.

Fryer L.S. and Kaiser G.D. (1979) *DENZ – A Computer Program for the Calculation of the Dispersion of Dense Gas Toxic or Explosive Gases in the Atmosphere,* Report SRD R 152, United Kingdom Atomic Energy Authority.

Gottschall C. (1997) *Establishing Acute Exposure Guideline Levels*, Chemical Health and Safety **4**(2): 38-41.

Hansen B.G., van Haelst A.G., van Leeuwen K. and van der Zandt P. (1999) *Priority Setting for Existing Chemicals: European Union Risk Ranking Method,* Environ. Tox. And Chem. **18**(4): 772-779.

Heidorn, C.J.A., Hansen, B.G. and Norager O. (1996) *IUCLID: A Database on Chemical Substances Information as a Tool for the EU-Risk-Assessment Program.* J.Chem. Inf. Comput. Sci. **36:** 949-954.

Holder B.W. and Munson L.H. (1996) *U.S. Department of Energy Participation in the Development of Emergency Response Planning Guidelines: The Program and Process,* Appl. Occup. Environ. Hyg. 11(4): 380-382.

Hushon J. and Kornreich M.R. (1984) in Axena J. (ed), *Hazard Assessment of Chemicals: Current Developments*, Academic Press, Vol. 3, 63-109.

Kalberlah F. and Winkelmann G. (1999) *The Concept of Acute Exposure Guideline Levels (AEGL) in Emergency Planning and Response,* Gefahrstoffe – Reinhaltung der Luft **59** (9): 321-326.

Lacoursiere J.P. Inc. (2002) *Rational for the Development of a List of Regulated Substances Under CEPA Section 200 and their Threshold Quantities*, Report Prepared for Environment Canada, Lacoursiere Inc, 35 Ave. Lemoyne, Repentigny, Quebec, Canada.
Also available at http://www.ec.gc.ca/CEPARegistry/documents/regs/e2_rationale/toc.cfm.

Lines I.G. and Deaves D.M. (1997) *The Implications of Dispersion in Low Wind Speed Conditions for Quantified Risk Assessment,* HSE Contract Research Report 133/1997, Suffolk: HSE Books.

Ludwig H.R., Cairelli S.G., and Whalen J.J. (1994) *Documentation for Immediately Dangerous to Life or Health Concentrations,* Report PB94-195047, Ohio: US Dept. of Health and Human Services.

Maddison T., Atkinson G. and Kinsman P. (1996) *The Assessment of Individual Risks From Fires in Warehouses Containing Toxic Materials,* I.Chem.E. Loss. Prev. Bulletin **132:** 29-34.

Markert F., Kozine I., Lauridsen K., Amendola A., and Christou M. (2001) *Sources and Magnitudes of Uncertainties in Risk Analysis of Chemical Establishments. First Insights from a European Benchmark Study*. Proceedings of the 10th International Symposium on Loss Prevention, 271-384.

McBride M. and Atkinson G. (2004) *Structural Fire Protection of Chemical Warehouses,* Industrial Safety Magazine **6**(1):14-16.

Munson L.H. and Holder B.W. (1991) *US Department of Energy Participation in the Development of Emergency Response Planning Guidelines: The Program and Process,* US Dept. of Energy Report DE92-004506, NTIS, Springfield, Virginia.

NAC, National Academy of Sciences (2000) *Appendix A: Priority Lists of Chemicals* http://www.nap.edu/openbook/.

NAC, National Advisory Committee (1997a) *Draft List of 78 Priority Chemicals for Acute Exposure Guideline Level (AEGL) Development,* Chemical Regulation Reporter **20**(50): 1655-1657.

NAC, National Advisory Committee (1997b) *EPA Notice of List of Priority Chemicals for Acute Exposure Guideline Level Development*, Chemical Regulation Reporter **21**(8): 236-237.

NRCCT, National Research Council Committee on Toxicology (1986) *Criteria and Methods for Preparing Emergency Exposure Guidance Level (EEGL), Short-term Public Emergency*

Guidance Level (SPEGL) and Continuous Exposure Guidance Level (CEGL) Documents, National Academy Press, Washington, DC: 1-34.

NRC, National Research Council Committee on Toxicology (2001) *Standard Operating Procedures for Developing Acute Exposure Guideline Levels for Hazardous Chemical,* Washington DC: National Academy Press.
(Also available at http://www.nap.edu/books/030907553X/html/.)

OECD, Organisation for Economic Co-Operation and Development (1986) *Existing Chemicals: Systematic Investigation, Priority Setting and Chemicals Review,* OECD, Paris.

Otway H. and Peltu M. (1985) *Regulating Industrial Risks: Science, Hazards and Public Protection,* Butterworth, London.

Petersen K.E. (1999) *The EU Model Evaluation Group,* J. Haz. Mat. **65:** 37-41.

Pittinger C.A., Brennan T.H., Badger D.A., Hakkinen P.J. and Fehrenbacher M.C. (2003) *Aligning Chemical Assessment Tools Across the Hazard-Risk Continuum,* Risk Analysis **23**(3): 529-535.

Rollin S.T. (2001) *First Batch of Final AEGLs Issued by National Research Council*, Chemical Regulation Reporter **25**(8): 390-392.

Ruden C. and Hansson S.O. (2003) *How Accurate are the European Union's Classifications of Chemical Substances,* Toxicology Letters **144:** 159-172.

Ruijten M. (2001) *Dutch Intitiative: Rotterdam Temporary Emergency Number Programme,* in: *Report of the OECD Expert Meeting on Acute Exposure Guideline Levels (AEGLs) Paris, 7-8 June 1999,* ENV/JM/MONO(2001)2 OECD, Paris.

Rusch G.M. *(*1993*)* The History and Development of Emergency Response Planning Guidelines, J. Haz. Mat. **33**: 193-202.

Rusch G.M., Garrett R., Tobin P., Falke E. and Po-Yung L. (2000) *The Development of Acute Exposure Guideline Levels for Hazardous Substances*, Process Safety Progress, **19** (2) 98-102.

Rusch G.M., Garrett R., Tobin P., Falke E. and Po-Yung L. (2002) *The Development of Acute Exposure Guideline Levels for Hazardous Substances,* Drug and Chemical Toxicology, 25 (4) 339-348.

Swanson M. and A. Socha A. (eds.) (1997) *Chemical Ranking and Scoring: Guidelines for Relative Assessments of Chemicals*, SETAC, Florida.

Trainor M.T., Macbeth R., Balmforth H. and Ridgway P. (2003) *Substance Prioritisation for the EU ACUTEX Project's 21 Acute Exposure Threshold Level Case Studies,* HSL Report RAS/03/17, HSE Information Centre, Broad Lane, Sheffield S3 7ZL, UK.

Trainor M., Macbeth R., Balmforth H. and Ridgway P. (2004) *Substance Prioritisation for the Development of EU Acute Exposure Toxicity Thresholds: Risk-Informed Decision Making,*: Proceedings of International Conference on Probabilistic Safety Assessment and Management (PSAM7), Berlin June 14-18, 2004, 192-197.

UN, United Nations (2001) *Recommendations on the Transport of Dangerous Goods: Model Regulations, Twelfth Revised Edition*, UN New York and Geneva.

van Haelst A.G. and Hansen B.G. (2000) *Priority setting for Existing Chemicals: Automated data selection route*, Environ. Tox. and Chem. **19**(9): 2372-2377.

Weiss M., Kordel W., Kuhnen-Clausen D., Lange A. and Klein W. (1988) *Priority Setting of Existing Chemicals*, Chemosphere **17**(8): 1419-1443.

Wood M. and Duffield, S. (2001) Proceedings from the *Workshop on Acute Exposure Guideline Levels (AEGLs), 28-30 May 2001*, Major Accident Hazards Bureau, Joint Research Centre, European Commission, Ispra, Italy.

11 GLOSSARY

Acute Exposure	Short term exposure, usually up to several hours duration.
AEGL	US Acute Emergency Guideline Level (see details in Appendix 2 of this report).
AETL	Acute Exposure Threshold Level.
Annex 1 Classification	A number of dangerous substances have a harmonised classification that is legally binding in the EU. These are listed in Annex 1 of the EU `Dangerous Substances Directive' (67/548/EEC). The classification is referred to as the substance's Annex 1 Classification.
Competent Authority:	The enforcing authority for the Seveso II directive in each EU Member State.
Corrosive substance	A Corrosive substance is one classified as such according to the EU 'Dangerous Substances Directive' (67/548/EEC).
Critical Review Panel:	The work of the ACUTEX project is being monitored by a Critical Review Panel comprising experts from major EU stakeholder groups including emergency planners, industry, Competent Authorities (the EU Member State enforcing authorities for the Seveso II Directive), toxicologists, and risk-related decision makers.
Hazard*	A situation with a potential for harm to people.
Irritant substance	An Irritant substance is one classified as such according to the EU 'Dangerous Substances Directive' (67/548/EEC).
LC_{50}	The LC_{50} for a particular species is the airborne concentration for a specified exposure period that will kill 50% of the exposed population.
MAHB	Major Accidents Hazards Bureau at the EU's Joint Research Centre: MAHB chairs the Critical Review Panel.
One-Shot Carcinogen	A substance that may cause cancer following a single, short-term exposure.
Physicochemical Properties	The inherent properties of a substance which influence potential exposure of people. For example, these might include vapour pressure, physical form, boiling point, and chemical stability.

Precursor	In this report, a precursor is a substance which is not a candidate for AETLs development, but which is of interest because a substance nominated for AETLs development is one of its reaction products.
Qualifying Quantity	Threshold quantity in tonnes of dangerous substances specified in the Seveso II Directive. The Qualifying Quantities define which chemical establishments fall within the scope of the Directive, either as `lower-tier' or `top-tier' sites. (See section 16.2 of this report for further details.)
Risk Phrase	A standard phrase used in the EU classification system for dangerous substances: it specifies a hazardous property of a substance. The risk phrases, and the criteria for their application, are defined in Annex IV of the EU `Dangerous Substances Directive' (67/548/EEC). See Appendix 5 of this report for additional information on the EU classification system.
Risk*	The likelihood (frequency) of a given degree of harm being suffered as a result of the realisation of specified hazards. That is to say, risk is a function of both likelihood and consequences. For example, risk may be expressed in terms of the likelihood of an accident at a site in which more than a specified number of people receive a specified dose or worse of toxic substances.
Toxic substance	A Toxic substance is one classified as such according to the EU 'Dangerous Substances Directive' (67/548/EEC).
Vapour	A gas that is below its 'critical temperature', the temperature above which it cannot be liquefied. In other words, a vapour is a gas that can be liquefied under pressure.
Very Toxic substance	A Very Toxic substance is one classified as such according to Council Directive 67/548/EEC, the 'Dangerous Substances Directive'.

*The definitions of hazard and risk are those used in the context of the control of major accident hazards from chemical plant.

12 APPENDIX 1: THE ACUTEX PROJECT

12.1 THE AIM OF ACUTEX

The aim of the ACUTEX project is to develop a methodology for establishing European Acute Exposure Threshold Levels (AETLs) for inhalation by people of toxic substances. As part of the methodology development, AETLs will be produced for 21 substances as case studies.

12.2 THE CONTEXT OF ACUTEX: MAJOR ACCIDENTS FROM CHEMICAL SITES AND THE SEVESO II DIRECTIVE

At this stage, AETLs development is in the context of the risks of major accidents from chemical sites and in particular their regulation through the EC Directive for the Control of Major Accident Hazards Involving Dangerous Substances (96/82/EC) [European Communities. Commission, 1997 & 2003], known as the Seveso II Directive. The Directive came into force in January 1997 and replaced the original Seveso Directive which was published by the CEC in 1982. The Directive is designed to be goal-oriented legislation with the aim of improving safety in the European chemical and associated industries. A description of its rationale and initial implementation is given in [Cassidy & Amendola, 1999]. The directive includes both accident prevention and mitigation. Here, accident mitigation refers to limiting the consequences of accidents through land-use planning and emergency planning including the provision of information to the public near sites. For sites with the potential to release toxic substances, decisions on accident prevention and mitigation are informed by estimations of dispersion distances for various foreseeable events based on the toxicology of the material involved and the extent and severity of likely harm.

It should be noted that broadening the context of AETLs development after the ACUTEX project has not been precluded. For example, possible areas of future interest include pipelines and dangerous goods transportation.

12.3 WHAT FORM AETLS WILL TAKE

AETLs will define the exposure conditions in terms of airborne concentration and exposure time that will produce a series of specified levels of harm to people for a number of toxic chemicals. The levels of harm have not yet been finalised, but they are likely to range from transient discomfort at the lower end of the scale, to severe long-lasting adverse health effects and, at the upper end of the scale, life threatening effects or death.

12.4 HOW AETLS MAY POTENTIALLY BE USED

It is considered that AETLs may potentially be used to aid decision making within EU Member States on emergency planning and land-use planning as appropriate in relation to Seveso II sites. The project does not, however, address how AETLs might be used in specific Member States as this is the responsibility of policy makers at Member State level. Rather it is intended that the ACUTEX project will:

- provide a broadly accepted, scientifically sound methodology for developing EU acute exposure thresholds which:
  - can be adapted, where appropriate, to the various national situations in land-use planning or emergency planning; and
  - will complement existing thresholds developed by Member States (or industry or other organisations); and
- through collaboration between toxicologists in the EU, and promotion of sharing data and expertise, reduce the overall cost of producing these thresholds.

12.5 THE SIGNIFICANCE OF THE DEGREE OF PRECAUTION IN TOXICOLOGICAL THRESHOLDS FOR EMERGENCY PLANNING AND LAND-USE PLANNING

The main source of uncertainty in the development of exposure threshold levels for humans is the paucity of toxicity data. In setting standards for safe levels of exposure to chemicals in, say, food or the workplace, a precautionary approach is used with 'uncertainty factors' applied to address issues such as extrapolation from data on animal exposure.

However, while a degree of precaution is necessary in developing thresholds for use in emergency planning in relation to potential accidents at chemical sites, overly cautious estimates can lead to, for example, inappropriate wide-scale evacuation and poor targeting of resources. Similarly, as regards land-use planning, overly cautious estimates can lead to, for example, inappropriate restrictions on land-use around chemical site. Therefore, an important issue being addressed in ACUTEX is the degree of precaution appropriate to employ in AETLs development taking into account the needs of Member States.

12.6 THE AETL METHODOLOGY IS INTENDED TO BUILD ON AND COMPLEMENT THE US AEGLS APPROACH

It is intended that the AETL methodology being developed under ACUTEX will complement the toxicological principles established in the US AEGLs program to create a complementary approach that also meets needs specific to users within the EU. Background information on AEGLs is given in Appendix 2. We note that the toxicological principles established in various EU Member State threshold methodologies will be considered in developing the AETL methodology.

Additionally, a specific consideration at EU level is the advantages or otherwise of joining the AEGLs program. This was discussed at a workshop held in May 2001 at the European Commission's Joint Research Centre [Wood & Duffield, 2001].

12.7 THE PROJECT PARTNERS AND TIMESCALE

The ACUTEX project has been approved under the EU's 'Fifth Framework' program of research. It has nine partner organisations in which government, industry, and researchers are represented. It is managed by:

- INERIS, Institut National de l'Environnement Industriel et des Risques, France.
- The other partners are:

- BgVV, The Federal Institute for Health Protection of Consumers and Veterinary Medicine, Germany;
- CEFIC, The European Chemical Industry Council;
- ECETOC, the European Centre for Ecotoxicology and Toxicology of Chemicals;
- HSE, The Health and Safety Executive, and HSL, The Health and Safety Laboratory, United Kingdom;
- ISPESL, The Institute for Prevention and Worker Safety, Italy;
- MAHB, The Major Accident Hazards Bureau of the European Commission's Joint Research Council;
- MRW, The Ministry of the Wallonne Region, Belgium; and
- UCL, The Catholic University of Louvain, Belgium.

Additionally, the work of the project is being monitored by a 'Critical Review Panel' comprising experts from major EU stakeholder groups including emergency planners, industry, Competent Authorities (the EU Member State enforcing authorities for the Seveso II Directive), toxicologists, and risk-related decision makers. The Critical Review Panel is chaired by the European Commission's Major Accident Hazards Bureau, MAHB.

The project started on 1st December 2002 and has a planned duration of 3 years.

13 APPENDIX 2: US ACUTE EXPOSURE GUIDELINE LEVELS (AEGLS)

The development of US Acute Exposure Guideline Levels (AEGLs) is described in [Rusch, 2003], [Rusch, 2000], [Gottschall, 1997], [EPA, 1997] and [EPA, 2001]. AEGLs are guideline levels for once-in-a-lifetime short-term exposures to airborne concentrations of acutely toxic substances. It is anticipated that they will be used in emergency planning and prevention as well as during real-time emergency response actions. This is in relation to the manufacture, processing, storage and transportation of chemicals and cleaning-up pollution. The context is both accidental and terrorist releases of chemical substances.

Three AEGL values are defined for a substance in terms of the airborne concentration at which the general population would experience the following:

AEGL 1	notable discomfort;
AEGL 2	irreversible effects or have impaired ability to escape;
AEGL 3	life-threatening effects or death.

The term general population is used to define a population that includes ‘susceptible’ but not ‘hyper-susceptible’ individuals. The AEGLs represent upper threshold values and apply to five specified exposure periods that range from 10 minutes to 8 hours.

AEGLs are developed under the US National Research Council's Committee on Toxicology by the National Advisory Committee for AEGLs for Hazardous Substances (NAC/AEGL). The NAC/AEGL is composed of representatives from US government, industry, medicine, academia and other organisations. It also includes representatives from the Dutch and German governments and an observer from the French government.

The NAC has identified 371 priority substances for AEGLs development [EPA, 2002]. They are to be developed at a rate of at least 30 substances per year initially, rising to 40 to 50 substances per year. In May 2002, 137 of these substances were listed as having high priority for AEGLs development [EPA, 2002]. If an AEGL cannot be developed for a priority substance because there is poor, or no, toxicity data, acute toxicity testing may be carried out. The guidelines for developing AEGLs are described in [NRC, 2001].

The AEGLs are published by the National Research Council National Academy of Sciences following a rigorous peer review process. The currently available AEGLs are given at http://www.umweltbundesamt.de/anlagen/AEGLWEB/index. At the end of September 2003 this listed:

- 18 substances with final AEGL values;
- 46 substances with interim AEGL values that had been established and initially reviewed and were awaiting final peer review and publication; and
- 33 substances with proposed AEGL values that had been published for public review following release from draft status.

14 APPENDIX 3: DEMONSTRATION OF SUBSTANCE RANKINGS USING HAZARD MEASURES ONLY

In order to demonstrate the effect of inclusion of Qualifying Quantities on the substance rankings obtained using the hazard measures only, we have considered the substances which formed the basis for selection of the preliminary 21 ACUTEX case study substances. This selection was described in [Trainor et al., 2003] and [Trainor et al., 2004]. These were the substances nominated by Member States in lists of '10 Substances of Interest' together with hydrazine which was included as an example of a Seveso II Named Carcinogen.

The following spreadsheet lists those substances which were in-scope for the case studies and are also in the scope advised for further AETLs development as described in section 3.1. No Irritants or Corrosives are in this list. The preliminary 21 ACUTEX case study substances are shown in bold italics at the top of the spreadsheet. The spreadsheet is followed by a description of the terminology used in it.

14.1 DEMONSTRATION OF SUBSTANCE RANKINGS FOR SOLIDS

For the 5 solid substances which had been nominated by Member States, the spreadsheet shows the rank obtained using the two hazard measures described in section 6.4:

- $1/4hLC_{50}$; and
- Qualifying Quantity / $4hLC_{50}$ (for Toxics and Very Toxics).

In both cases, 1 is the highest rank or greatest hazard.

14.2 DEMONSTRATION OF SUBSTANCE RANKINGS FOR FLUIDS (LIQUIDS AND VAPOURS)

As described in section 6.3, the spreadsheet gives a very crude demonstration of the effect of Qualifying Quantity on rank for the 31 fluid substances listed. The spreadsheet gives the indicative hazard measure

$$VP/ 4hLC_{50}$$

described in section 6.3.3, and shows how the substances are ranked according to this measure. It also shows how the substances are ranked if the measure

$$\text{Top-tier Quantifying Quantity} \times VP/ 4hLC_{50}$$

is used instead. In both cases, 1 is the highest rank or greatest hazard.

SUBSTANCES

	Name	CAS #	In Scope	In Scope	Risk phrases	10 Interest nom	21 Case Studies	Approximate 4 h LC50 (mg/l)	VP @ 20C (Pa)
1	***Hydrazine***	302-01-2	Y - Sev (NC)	CARC	R45 R10 R23/24/25 R34 R43 R50/53 (Named Carc)		Y	3.34E-01	
2									
3	***Acrylonitrile***	107-13-1	Y - Sev	T (An1)	R45 R11 R23/24/25 R37/38 R41 R43 R51/53	Y	Y	2.32E-01	11533.3
4	***Allylamine***	107-11-9	Y - Sev	T (An1)	R11 R23/24/25 R51/53	Y	Y	6.80E-01	25786.7
5	***Ammonia***	7664-41-7	Y - Sev	T (An1)	R10 R23 R34 R50	Y	Y	1.47E+00	835755.4
6	***Aniline***	62-53-3	Y - Sev	T (An1)	R20/21/22 R40 R48/23/24/25 R50	Y	Y	7.60E-01	62.7
7	***Carbon disulphide***	75-15-0	Y - Sev	T (An1)	R11 R36/38 R48/23 R62 R63	Y	Y	5.02E+00	39361.3
8	***Chlorine***	7782-50-5	Y - Sev	T (An1)	R23 R36/37/38 R50	Y	Y	1.33E-01	677756.5
9	***Dichlorophenyl isocyanate***	102-36-3	Y - Sev	T+(SC)	R42 self classified R26?	Y	Y	1.57E-01	SOLID
10	***Ethylene oxide***	75-21-8	Y - Sev	T (An1)	R45 R46 R12 R23 B77R36/37/38	Y	Y	1.45E+00	147552.3
11	***Hydrogen chloride***	7647-01-0	Y - Sev	T (An1)	R23 R35	Y	Y	4.84E-01	4264125.6
12	***Hydrogen fluoride***	7664-39-3	Y - Sev	T+(An1)	R26/27/28 R35	Y	Y	1.42E-01	121451.8
13	***Hydrogen sulphide***	7783-06-4	Y - Sev	T+ (An1)	R12 R26 R50	Y	Y	7.10E-01	1764037.8
14	***Methanol***	67-56-1	Y - Sev	T (An1)	R11 R23/24/25 R39/23/24/25	Y	Y	1.50E+02	12898.7
15	***Nitrogen dioxide***	10102-44-0	Y - Sev	T+(An1)	R26 R34	Y	Y	9.77E-02	96040.9
16	***Oxybenzene (phenol)***	108-95-2	Y - Sev	T (An1)	R24/25 R34	Y	Y	9.80E-01	SOLID
17	***Phorate***	298-02-2	Y - Sev	T+(An1)	R27/28	Y	Y	2.71E-03	1.1
18	***Phosgene***	75-44-5	Y - Sev	T+(An1)	R26 R34	Y	Y	7.46E-03	157222.8

	Name	CAS #	In Scope	In Scope	Risk phrases	10 Interest nom	21 Case Studies	Approximate 4 h LC50 (mg/l)	VP @ 20C (Pa)
19	***Phosphorus trichloride***	7719-12-2	Y - Sev	T+(An1)	R14 R26/28 R35 R48/20	Y	Y	2.92E-01	13741.2
20	***Propionitrile***	107-12-0	Y - Sev	T (SC)	Self classification= R26	Y	Y	9.37E-02	4892.0
21	***Sulphur dioxide***	7446-09-5	Y - Sev	T (An1)	R23 R34	Y	Y	1.49E+00	337430.8
22	***Toluene diisocyanate***	26471-62-5	Y - Sev	T+(An1)	R26 R36/37/38 R40 R42/43 R52/53	Y	Y	1.45E-02	1.4
23									
24	Acetone cyanohydrin	75-86-5	Y - Sev	T+(An1)	R26/27/28 R50/53	Y		2.48E-01	29.5
25	Acrolein	107-02-8	Y - Sev	T+(An1)	R11 R24/25 R26 R34 R50	Y		3.74E-02	29349.6
26	Acrylamide	79-06-1	Y - Sev	T (An1)	R45 R46 R20/21 R25 R36/38 R43 R48/23/24/25 R62	Y		1.18E-01	SOLID
27	Carbofuran	1563-66-2	Y - Sev	T+(An1)	R26/28 R50/53	Y		HSDB = 3.00E-02	SOLID
28	Carbonyl sulphide	463-58-1	Y - Sev	T+(SC)	Self classification=R26	Y		s = 1.00E+00	1103541.3
29	Chlorine dioxide	10049-04-4	Y - Sev	T+(An1)	R6 R8 R26 R34 R50	Y		AEGL = 1.00E-01	144942.0
30	Ethylene dibromide	106-93-4	Y - Sev	T (An1)	R45 R23/24/25 R36/37/38 R51/53	Y		1.45E+00	1354.9
31	Fluorine	7782-41-4	Y - Sev	T+(An1)	R7 R26 R35+F13	Y		1.25E-01	
32	Formaldehyde	50-00-0	Y - Sev	T (An1)	R23/24/25 R34 R40 R43	Y		4.25E-02	425954.1
33	Hydrogen cyanide	74-90-8	Y - Sev	T+(An1)	R12 R26 R50/53	Y		4.78E-02	81885.2
34	Methyl bromide	74-83-9	Y - Sev	T (An1)	R23/25 R36/37/38 R48/20 R50 R59 R68	Y		7.91E-01	177188.9
35	Methyl chloroacetate	96-34-4	Y - Sev	T (An1)	R10 R23/25 R37/38 R41	Y		3.76E+00	732.1
36	Methyl chloroformate	79-22-1	Y - Sev	T (An1)	R11 R23 R36/37/38	Y		8.66E-02	11247.2
37	Methyl iodide	74-88-4	Y - Sev	T (An1)	R21 R23/25 R37/38 R40	Y		1.37E+00	44326.4
38	Nickel tetracarbonyl (nickel carbonyl)	13463-39-3	Y - Sev	T+(An1)	R61 R11 R26 R40 R50/53	Y		8.61E-03	4280.0

	Name	CAS #	In Scope	In Scope	Risk phrases	10 Interest nom	21 Case Studies	Approximate 4 h LC50 (mg/l)	VP @ 20C (Pa)
39	Paraquat dichloride	1910-42-5	Y - Sev	T+(An1)	R24/25 R26 R36/27/38 R48/25 R50/53	Y		1.50E-03	SOLID
40	Phenyl mercaptan	108-98-5	Y - Sev	T (SC)	Self classification=R26	Y		1.29E-01	44326.4
41	Terbufos	13071-79-9	Y - Sev	T+(An1)	R27/28	Y		2.34E-02	?

	Name	VP/LC50			Quantity x VP/LC50			1 / LC50 Solids		
		Actual	Scaled	Rank	Actual	Scaled	Rank	Actual	Scaled	Rank
1	***Hydrazine***									
2										
3	***Acrylonitrile***	49682.98	602.3934	20	9936596	4185.51	19			
4	***Allylamine***	37903.64	459.572	22	7580728	3193.167	20			
5	***Ammonia***	568441.9	6892.212	12	1.14E+08	47888.01	4			
6	***Aniline***	82.47596	1	31	16495.19	6.948133	28			
7	***Carbon disulphide***	7837.66	95.02963	24	1567532	660.2785	23			
8	***Chlorine***	5108094	61934.34	4	1.28E+08	53791	3			
9	***Dichlorophenyl isocyanate***	S	S			S		6.37	6.25	4
10	***Ethylene oxide***	101481.7	1230.439	18	5074083	2137.314	22			
11	***Hydrogen chloride***	8805913	106769.4	3	2.2E+09	927310.3	1			
12	***Hydrogen fluoride***	852885.5	10341.02	10	17057709	7185.077	14			
13	***Hydrogen sulphide***	2484560	30124.66	5	49691205	20931.01	6			
14	***Methanol***	85.88429	1.041325	30	17176.86	7.235265	27			
15	***Nitrogen dioxide***	982579.8	11913.53	9	19651596	8277.679	13			

	Name	VP/LC50			Quantity x VP/LC50			1 / LC50 Solids		
		Actual	Scaled	Rank	Actual	Scaled	Rank	Actual	Scaled	Rank
16	***Oxybenzene (phenol)***	S	S			S		1.02	1	5
17	***Phorate***	412.9308	5.006681	26	8258.616	3.478708	30			
18	***Phosgene***	21074828	255526.9	1	15806121	6657.881	15			
19	***Phosphorus trichloride***	47080.05	570.8336	21	941601	396.6228	24			
20	***Propionitrile***	52206.38	632.989	19	10441276	4398.092	17			
21	***Sulphur dioxide***	226944.6	2751.646	15	45388930	19118.8	7			
22	***Toluene diisocyanate***	94.21236	1.142301	29	9421.236	3.968429	29			
23										
24	Acetone cyanohydrin	118.7023	1.439236	28	2374.047	1	31			
25	Acrolein	785308.9	9521.67	11	15706177	6615.783	16			
26	Acrylamide	S	S			S		8.48	8.31	3
27	Carbofuran	S	S			S		33.3	32.7	2
28	Carbonyl sulphide	1103541	13380.16	8	22070826	9296.711	12			
29	Chlorine dioxide	1449420	17573.85	7	28988404	12210.54	10			
30	Ethylene dibromide	935.6522	11.34454	25	187130.4	78.8234	25			
31	Fluorine	No VP	No VP			No VP				
32	Formaldehyde	10012438	121398.3	2	5.01E+08	210872.8	2			
33	Hydrogen cyanide	1713554	20776.4	6	34271071	14435.72	9			
34	Methyl bromide	223959	2715.446	16	44791800	18867.28	8			
35	Methyl chloroacetate	194.8408	2.362395	27	38968.16	16.41424	26			
36	Methyl chloroformate	129838.2	1574.254	17	25967630	10938.13	11			
37	Methyl iodide	32305.84	391.7	23	6461168	2721.584	21			
38	Nickel tetracarbonyl (nickel carbonyl)	497203.7	6028.468	13	9944074	4188.66	18			
39	Paraquat dichloride	S	S			S		666.67	653.6	1
40	Phenyl mercaptan	344836.3	4181.052	14	68967263	29050.51	5			
41	Terbufos	No VP	No VP			No VP				

	Name	Quantity / LC50 (Solids)			Country Total Y response
		Actual	Scaled	Rank	
1	***Hydrazine***				
2					
3	***Acrylonitrile***				**5**
4	***Allylamine***				**1**
5	***Ammonia***				**4**
6	***Aniline***				**1**
7	***Carbon disulphide***				**2**
8	***Chlorine***				**6**
9	***Dichlorophenyl isocyanate***	127.6528	1	5	**1**
10	***Ethylene oxide***				**2**
11	***Hydrogen chloride***				**6**
12	***Hydrogen fluoride***				**6**
13	***Hydrogen sulphide***				**6**
14	***Methanol***				**1**
15	***Nitrogen dioxide***				**2**
16	***Oxybenzene (phenol)***	204.0166	1.598215	4	**1**
17	***Phorate***				**1**
18	***Phosgene***				**4**
19	***Phosphorus trichloride***				**1**
20	***Propionitrile***				**1**
21	***Sulphur dioxide***				**3**
22	***Toluene diisocyanate***				**3**
23					
24	Acetone cyanohydrin				**1**

	Name	Quantity / LC50 (Solids)			Country Total Y response
		Actual	Scaled	Rank	
25	Acrolein				**1**
26	Acrylamide	1688.239	13.22524	2	**1**
27	Carbofuran	667	5.21	3	**1**
28	Carbonyl sulphide				**1**
29	Chlorine dioxide				**1**
30	Ethylene dibromide				**1**
31	Fluorine				**1**
32	Formaldehyde				**1**
33	Hydrogen cyanide				**1**
34	Methyl bromide				**1**
35	Methyl chloroacetate				**1**
36	Methyl chloroformate				**1**
37	Methyl iodide				**1**
38	Nickel tetracarbonyl (nickel carbonyl)				**1**
39	Paraquat dichloride	13330.37	104.4268	1	**1**
40	Phenyl mercaptan				**1**
41	Terbufos				**1**

SPREADSHEET TERMINOLOGY

Table Heading	Assoc. Codes	Description
Name	-	Name of the substance. This may not be the synonym by which the substance is known by some Competent Authorities. Names in ***Bold Italics*** indicate that the substance has been selected as one of the preliminary 21 AETL case-study substances. Names in *Italics* indicate that the substance was proposed by a Competent Authority as one of their intial 10 substances of interest.
CAS #	-	The Chemical Abstracts Service Registry number for the substance to assist in identification of substances known by more than one name. (http://www.cas.org).
In Scope	Y - SEV	Yes, In scope for development of AETL under Seveso II.
	Y - SEV (NC)	Named Carcinogen under Seveso II.
	Y - MIS	Yes, In scope for development of AETL on the basis of approximate 4hLC50 because potentially MIS classified in Annex 1.
	Y - XC	Yes, In scope for development of AETL because corrosive or irritant.
	N	No, Out of scope.
	N/A	Not applicable, This is a precursor substance which has not been nominated for AETLs development.
Risk phrases		Risk phrases as defined in Annex IV to the EU `Dangerous Substances Directive (67/548/EEC).
	R6	Explosive with or without contact with air
	R7	May cause fire.
	R8	Contact with combustible material may cause fire
	R10	Flammable.
	R11	Highly flammable.
	R12	Extremely flammable.
	R14	Reacts violently with water.
	R20	Harmful by inhalation.
	R21	Harmful in contact with skin.
	R22	Harmful if swallowed.
	R23	Toxic by inhalation.
	R24	Toxic in contact with skin.
	R25	Toxic if swallowed.
	R26	Very Toxic by inhalation.
	R27	Very Toxic in contact with skin.
	R28	Very Toxic if swallowed.
	R34	Causes burns.
	R35	Causes severe burns.
	R36	Irritating to eyes.
	R37	Irritating to respiratory system.
	R38	Irritating to skin.
	R39/23/24/25	Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.
	R40	Limited evidence of a carcinogenic effect.
	R41	Risk of serious damage to eyes.
	R42	May cause sensitization by inhalation.
	R43	May cause sensitization by skin contact.
	R45	May cause cancer.

	R46	May cause heritable genetic damage.
	R48/20	Harmful: danger of serious damage to health by prolonged exposure through inhalation.
	R48/23	Toxic: danger of serious damage to health by prolonged exposure through inhalation.
	R48/23/24/25	Toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed.
	R48/25	Toxic:danger of serious damage to health by prolonged exposure if swallowed.
	R49	May cause cancer by inhalation.
	R50	Very Toxic to aquatic organisms.
	R51	Toxic to aquatic organisms.
	R52/53	Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
	R53	May cause long term adverse effects in the aquatic environment.
	R59	Dangerous for the ozone layer.
	R61	May cause harm to the unborn child.
	R62	Possible risk of impaired fertility.
	R63	Possible risk of harm to the unborn child.
	R65	Harmful: may cause lung damage if swallowed.
	R66	Repeated exposure may cause skin dryness or cracking.
	R67	Vapours may cause drowsiness and dizziness.
	R68	Possible risk of irreversible effects.
	REV	Revised classification likely to be included in 29th ATP.
10 Interest Nom		Nominated substance from a Competant Authority in list of '10 Substances of Interest'
	Y	Yes
Tox risk significant	N	Toxicity is not the principal hazard associated with the substance. Given for in-scope substances only.
Approximate 4h LC50 (mg/L)	-	4 hour Lethal Concentration 50% fatality. (Derived from UK SLOD DTLs on http://www.hse.gov.uk/hid/HAZTOX.HTM). If no SLOD DTL is available then a 4-hour LC50 value is calculated or listed from another stated source: AEGL, ACGIH, HSDB etc. see notes below. Alternatively S (special) indicates other information has been used. Values are APPROXIMATE. `No' indicates where no data has been found.
VP @ 20^{o}C		Vapour Pressure (Pa) at 20°C. Calculated from the American Institute of Chemical Engineers (AIChE) Design Institute for Physical Properties (DIPPR) database for gases/liquids with critical temperature greater than ambient temperature (20°C)
VP/LC50		
Actual		Vapour Pressure divided by the 4h LC50 (mg/L).
Scaled		Above quantity scaled to the lowest value in current list of substances.
Rank		Corresponding rank of substance where 1 is highest.
Quantity x VP/LC50:		
Actual		Above value multiplied by the Top Tier Qualifying Quantity. (Very Toxic = 20 te; Toxic = 200 te. The named substances are: Chlorine (25 te); Formaldehyde (50 te); Hydrogen chloride (250 te); Ethylene oxide (50 te); Toluene diisocyanate (100 te); Phosgene (0.75 te); Methanol = 5000 te. No Vapour Pressure can be calculated for the named substance Fluorine.
Scaled		Above scaled to the lowest value in current list of substances.

Rank		Corresponding rank of substance where 1 is highest.
1 / LC50 Solids Actual Scaled Rank		1 / LC50 for solids. Above scaled to the lowest value in current list of substances. Corresponding rank of substance where 1 is highest.
Quanitity / LC50 (Solids): Acutal Scaled Rank		 Top Tier Qualifying Quantity (see above) divided by LC50 for solids. Above scaled to the lowest value in current list of substances. Corresponding rank of substance where 1 is highest.
Country	Total Y response	Sums the "Yes" responses for the proposed inclusion of a substance by each of the Competent Authorities in their lists of '10 Substances of Interests'.

NOTE: MEL (8hr TWA)= UK Maximum Exposure Limit [HSE, 2002].

NOTE: ACGIH TLV= American Conference of Governmental Industrial Hygienists (Details are in their CD-ROM: `Documentation of the TLVs and BEIs and Other Wordwide Occupatrional Exposure Values', 2002.)

NOTE: OES (8hr TWA)= UK Occupational Exposure Standard, 8-hour TWA [HSE, 2002].

NOTE: AEGL= US Acute Exposure Guideline Levels (up to date information on AEGLs can be found at http://www.umweltbundesamt.de/anlagen/AEGLWEB/).

NOTE: HSDB= US Hazardous Substances Database at http://toxnet.nlm.nih.gov

NOTE: MSDA = Material Safety Data Sheet (from Air Liquide website: http://www.airliquide.com/safety/msds/en/index.htm)

NOTE: ESR RAR = EU Existing Substances Regulation Risk Assessment Report

15 APPENDIX 4: APPROACHES TO SUBSTANCE PRIORITISATION

As background to the development of the AETLs substance prioritisation methodologies, we looked at approaches to substance prioritisation adopted elsewhere. The material we considered is described in this Appendix as follows:

- Firstly we outline four publications giving reviews of, or guidance on, substance prioritisation approaches. Substance prioritisation is a well developed field and we found that these general reviews and guidance provided a valuable starting point from which to develop the AETLs prioritisation methodologies.

- Secondly we give a brief overview of substance prioritisation approaches developed in the context of generating toxicological information for use in the control of major accidents from chemical plant. We did not find any information published in sufficient detail to allow us to draw upon it in developing the AETLs prioritisation methodologies.

- Finally we outline two EU prioritisation methodologies developed in other contexts. These were particularly useful to us in indicating how stakeholder consultation operates at EU level, some of the practical issues involved in data gathering and checking, and the importance accorded to disseminating the details of the methodologies.

15.1 REVIEWS OF APPROACHES TO SUBSTANCE PRIORITISATION

Substance prioritisation is important to various aspects of risk regulation and is widely carried out. In this section we outline four reviews of, or guidance on, priority setting approaches.

15.1.1 The 1984 Review by Hushon and Kornreich

[Hushon and Kornreich, 1984] consider scoring systems used to `rank compounds according to their relative capacity for inflicting adversity upon man and his environment. Scoring is usually viewed as a screening tool to assist at an early stage of the hazard assessment process in setting priorities among chemical substances that should receive more intensive scientific review before being selected for research, testing, or regulation.' Some 30 scoring methods are summarised. Aspects discussed include the following:

- Grouping of substances into groups or classes is an optional and often controversial step. Substances within a group may vary widely making it difficult or meaningless to assign a single score. However it can be beneficial: an example is cited where substances were selected after first grouping them according to structural classes.
- A team approach is often desirable for assigning scores since expertise is needed in a number of disciplines. Some of the knowledge on which a score is based will be objective while some will be subjective; some will be quantitative while some will be qualitative.
- Criteria must be defined in terms of parameters for which data are readily available for large numbers of substances.

15.1.2 The 1986 OECD Expert Groups' Guidance for the Development and Use of Priority Setting Processes

The 1986 OECD expert groups' publication [OECD, 1986] provides `guidance for the development and use of priority setting processes to select existing chemicals for further investigation of their potential effects on human health and the environment'. It was prepared as part of their remit to assist member countries in the 'rational, pragmatic and cost-effective' selection of existing chemicals.

Aspects of substance prioritisation highlighted include the following:

- It is necessary to identify the purpose and scope of any priority setting exercise. This may imply definition of practical constraints, legislative/administrative considerations and scientific/technical considerations.
- The outputs of a selection exercise are the group of selected priority substances, non-selected/lower-priority substances, and non-relevant substances which are either outside the scope of the selection exercise or are substances for which data are adequate.
- Expert judgment is required throughout the process – at no stage is it purely mechanical.
- The process may be considered as having four stages: compilation, screening, refinement and review. The quantity and complexity of information increase throughout these stages. However, the initial stages may be bypassed if the number of substances involved is such that they can be handled with the available resources at a later stage. The number of candidate substances may also influence the manner in which information is searched for and applied.
- Care must be taken not to generate `false positives' (i.e. selection of substances which are not of high concern) or `false negatives' (i.e. missing out substances of concern).
- The process should be repeated after some interval in order to rectify possible errors, update the data and improve the selection methods.

The publication also lists about 60 systems for selecting and establishing priorities: these are all the systems which had been cited in recent literature. Summaries are given of 15 of these systems; they were chosen because they were in current use in OECD member countries, or presented especially interesting aspects of selection or priority setting.

15.1.3 The 1994 Review by Davis, Swanson and Jones

[Davis et al., 1994] evaluate 38 systems for risk-based ranking and scoring of substances. The systems are considered to fall into two major types: those which rank substances, and those which categorise them (for instance, in high medium or low concern categories). They note that the systems `are typically intended to be fairly simple and quick methods for determining the health and environmental hazards posed by the use and release of chemical substances. Although not intended to provide a quantitative assessment of risk, the majority of the systems reviewed do rely on the basic principles of risk assessment. … Most chemical ranking systems include measures of both toxicity and exposure and, in this way, are similar to quantitative risk assessment methods. The major difference is the extent to which the exposure assessment is performed.'

15.1.4 The 1995 SETAC Workshop on Chemical Ranking and Scoring

An international workshop organized by the Society of Environmental Toxicology and Chemistry, SETAC, in 1995 produced a framework for chemical ranking and scoring within the context of chemical risk assessment and management. The proceedings of the workshop are published in [Swanson and Socha, 1997]. Here, chemical ranking and scoring is defined as `a tool for assessing chemicals by considering health effects, environmental effects or other hazards, persistence, and exposure. Chemical ranking and scoring either produces a relative ranking of chemicals or assigns chemicals to specific groups or categories.' It is noted that although chemical ranking and scoring systems are not generally considered equivalent to chemical risk assessment, their information needs and complexity `may be thought of as a continuum from simple, single-factor screening to quantitative risk assessment.' This is explored further in [Pittinger et al., 2003]. The workshop proceedings give examples of existing chemical ranking and scoring schemes for a wide range of applications. Their use by governments, industry and academia is described for applications including regulation and risk management, priority setting for testing and assessment of chemicals, setting priorities for research and development, and determining chemical data needs.

According to the proceedings, the most common existing chemical ranking and scoring schemes may be classified under four broad classes or hybrids of them:

1) simple categorisation based on expert judgment;
2) decision rule where chemicals are sorted into groups based on criteria and using decision rules;
3) endpoint scoring, with or without numerical aggregation; and
4) generic risk calculation.

It is noted that within each category there are variations. A further breakdown of systems into types is also given with examples. The advantages and disadvantages of the four broad classes are discussed. For example, endpoint scoring and generic risk calculation type schemes are typically more complex and data resource intensive than decision rule and simple categorisation schemes, they usually require more time and resources to develop and use, and as a result of their complexity may be less transparent. In comparison, decision and simple categorisation schemes tend to be more transparent and can be developed and applied quickly, but may suffer from a lack of widespread acceptance.

A set of principles are given for the development of any new chemical ranking and scoring systems. In summary, it is stated that a new system should:

- have a clearly defined purpose;
- include both effect and exposure data;
- acknowledge and assess uncertainty;
- acknowledge the role of professional judgement;
- consider effects relevant to the goals;
- recognise the role of valuation in aggregation and weighting of different endpoints;
- have transparent methods and outputs;
- be neutral to data availability, unless a bias is consistent with the intended use;
- be able to deal with extreme data variability across chemicals;
- assess similar effects or exposure categories consistently across tiers;
- preserve critical information;
- specify data selection guidelines;
- be theory and data driven;

- include sensitivity analysis;
- be consistent with any pre-selection of chemicals; and
- consider the impacts of scaling.

Additionally, a four step generic framework for chemical ranking and scoring systems is given:

1) Goal definition and scoping.
2) Indicator selection: identifying the type and amount of data needed.
3) Ranking and scoring based on agreed-upon principles.
4) Output and presentation: an effort must be made to make the process transparent and to communicate important information to the user.

15.2 SUBSTANCE PRIORITISATION FOR THE DEVEOPMENT OF TOXICOLOGICAL INFORMATION USED IN THE CONTEXT OF MAJOR ACCIDENTS FROM CHEMICAL PLANT

A range of toxicological information is in use in EU Member States for either emergency planning or land-use planning purposes in the context of major accidents from chemical plant. (One of the planned outcomes of the ACUTEX project is a publication describing these.) We have not found any published information on substance prioritisation for the development of this information which is in sufficient detail to allow us to draw upon it in developing the methodologies for prioritizing substances for AETLs development.

The following two sub-sections describe the approaches used to prioritise substances for the development of AEGLs and ERPGs. The remaining toxicological information was either developed for other purposes so that their prioritisation is not relevant here, was developed for all the substances of interest (i.e. prioritisation was not involved), or, so far as we are aware, has very limited or no published details on substance prioritisation. A brief breakdown follows.

Toxicity information used in the context of the control of major accidents from chemical plant is considered in: [Alexeeff et al., 1991], [Rusch, 1993], [Holder & Munson, 1996] and [Kalberlah & Winkelmann, 1999]. In addition to AEGLs and ERPGs, toxicity information listed includes the following:

- US Immediately Dangerous to Life or Health, IDLH, values [Alexeeff et al., 1989]: these were developed in the context of respirator selection for workers.
- US Emergency Exposure Guidance Levels, EEGLs and US Short Term Public Emergency Guidance Levels, SPEGLs [NRCCT, 1986]: these were developed in the context of military operations and space travel.
- Various occupational exposure guidelines developed in the context of worker safety (many for long-term rather than short-term exposures) including short-term exposure limits (TLV-STELs) or time-weighted averages (TLV-TWAs) and ceiling limits developed by the American Conference of Governmental Industrial Hygienists [ACGIH, 1986].
- US Temporary Emergency Exposure Limits, TEELs [Craig et al., 2000]: these are approximations to ERPGs and are produced for substances of interest for ERPG or AEGL development in order to serve as temporary guidance.
- Emergency Exposure Indices, EEIs: these are for use as guidance on the potential health effects from accidental chemical releases from chemical installation. Guidelines for developing EEIs were developed by the European Chemical Industry Ecology and Toxicology Centre (ECETOC) [ECETOC, 1991]. However ECETOC does not have a

program of EEI development, rather it is intended that chemical industries may develop EEIs as necessary using the ECETOC guidelines.

At EU Member State level, other relevant toxicity information includes:

- French Thresholds of Lethal Effects, SEIs, and Thresholds of Irreversible Effects, SELs [Pichard, 2001]: these are used for land-use planning purposes. They were initially developed for 26 substances prioritised according to those most frequently included in the hazard studies of installations carried out by industry.
- UK Specified Levels of Toxicity, SLOTs [Fairhurst & Turner, 1993]: these are used by HSE (part of the UK Competent Authority for the Seveso Directive) to give advice on land-use planning in the vicinity of chemical site. They have been produced for all substances of interest – namely the substances which HSE has 'screened' for their potential to pose off-site risks when giving land-use planning advice or assessing Seveso safety reports prepared by industry.
- Dutch Emergency Guideline Levels [Ruijten, 2001]: these were developed for 280 priority substances identified on the basis of: production; storage; transportation; volatility; and toxicity.

15.2.1 Substance Prioritisation for US Emergency Response Planning Guides (ERPGs)

The US Emergency Response Planning Guides, ERPGs are being developed by the American Industrial Hygiene Association as planning and emergency response guidelines in the context of exposure of the public to acutely toxic chemicals resulting from accidental releases. They are described in [Rusch, 1993], [Holder & Munson, 1996] and [Munson & Holder, 1991]. In 2002, ERPGs had been produced for about 100 chemicals[32].

Substance prioritisation for ERPGs is described in [Rusch, 1993]. Candidate chemicals are selected by a review committee formed of scientific representatives from member companies. The selection criteria considered include:

- quantities produced;
- the number of people and sites using the substance;
- the number of companies using the substance;
- whether it appears to be a highly toxic substance; and
- the physical properties of the chemical (i.e. whether gas or volatile liquid which could lead to widespread distribution, or a solid with limited potential for dispersion).

So far as we are aware, details of how these selection criteria are considered are not published.

Additionally, the chemicals on two existing lists are given consideration, namely the `Hazardous Substance List from SARA Title III' and the `OSHA list of Highly Hazardous Chemicals'.

[32] The chemicals with ERPGs are listed on the website of The American Industrial Hygiene Association at http://www.aiha.org/PublicationsAdvertising/html/POerpgweels.htm. (To access this it is necessary to go via the main site as some parts of the site are restricted entry.)

Selection of the first 6 substances is described in [Munson & Holder, 1991]. They describe the use of a prioritisation scale of 1 to 5 where 1 was the most urgent and 5 the least urgent.

15.2.2 Substance Prioritisation for US AEGLs Development

The US Acute Exposure Guideline Levels, AEGLs, are outlined in Appendix 2. Substance prioritisation for AEGLs development is described in [NAC, 2000], [EPA, 2001], [Gottshall, 1997] and [Rush et al., 2000]. To date, two priority lists have been published. Points of note include:

- The priority substances reflect the priorities of the organisations involved in AEGLs development.
- The priority substances are subject to change based on the changing priorities of the organisations involved in AEGLs development and of the NAC/AEGL committee.
- Prioritisation is independent of the availability of toxicological data. Where there is poor or no data, the substance may be subjected to appropriate acute testing [EPA, 2001].

The first list of 85 priority substances was published in 1997 [NAC, 1997b]. This list identified those substances of highest priority across the US government agencies represented on the NAC as selected by the NAC/AEGL committee. [NAC, 2000] identifies which priority substances relate to which agency. As described in [EPA, 2001], the prioritisation process began by integrating the individual lists of priority substances from the US government agencies represented on the NAC. These individual lists were based on assessments of the:

- hazards,
- potential exposure,
- risk, and
- relevance of substances to the agency's work program.

From these individual lists, a master list of approximately 1,000 substances was initially produced. From this master list a list of approximately 400 higher priority chemicals was tentatively identified. This was used to identify an initial draft list of 78 priority chemicals published in [NAC, 1997a] and subsequently the published list of 85 substances. [Gottshall, 1997] notes that the draft master list drawn from the individual lists reflected a fair distribution of each organization's priorities and that prioritisation focused on the top 20% of this list. So far as we are aware, details of the assessments underpinning the individual lists are not published. In particular, we are not aware of any details on prioritisation in relation to off-site risks from chemical sites. However it is noted [Rollin, 2001] that at the request of the US Army, old chemical warfare agents were prioritised because of the need to protect workers disarming ageing weapons.

The second list of 371 priority substances for AEGLs development identified by the NAC was published in 2002. It includes 137 substances considered to be a high priority based on 'considerations of toxicity, volatility, presence on numerous organization chemical lists, and other factors' [EPA, 2002]. The list was selected from the original master list together with new candidate substances proposed by participants in the AEGLs program (various US federal agencies and organisations and some OECD countries). Priority lists for the AEGLs are longer than are predicted for an AETLs program because the AETL priority scheme recommendations relate only to substances of interest in the context of Seveso II, whereas AEGLs are being developed for chemicals of interest not just in relation to accidental releases from major chemical plants, for example in the areas of transport or warfare.

15.3 SUBSTANCE PRIORITISATION CARRIED OUT IN AN EU CONTEXT

Below we give an overview of two EU substance prioritisation methodologies developed in other contexts: danger to the aquatic environment, and existing substances. A noteworthy feature of both is the high level of detail in the published information on them.

15.3.1 EU Prioritisation of Substances Dangerous to the Aquatic Environment: The 'COMMPS' Scheme.

Under the EU `Water Framework Directive' (Directive PE-CONS 3639/00) Member States are required to establish a monitoring network for a named list of substances. The EU prioritization methodology developed to select these substances is called the Combined Monitoring-Based and Modelling-Based Priority Setting Scheme, COMMPS. COMMPS is based on the risks substances pose to the aquatic environment and to human health via the aquatic environment; it is described in [European Commission, EU 1999]. The development of COMPSS included consulting experts from Member States, industry and elsewhere; in particular a working paper was prepared for comment and discussion.

In support of COMPSS, a database was set up to hold monitoring data from the Member States and the European Union of National Associations of Water Suppliers and Waste Water Services. During a checking stage defective or inappropriate data was replaced or deleted. For example, one Member State had supplied data with the wrong concentration units.

658 candidate substances were compiled from EU and international lists together with additional substances identified from the monitoring data supplied by the Member States.

Several ranked lists of substances were then drawn up in a step-wise process considering exposure indices, effect indices, and computation of a risk-based priority index. Human health scores within the effect indices are based on substances' risk phrases. Substances may appear on more than one of these ranked lists. For example, there is a monitoring-based and a separate modelling-based list for organic substances in the aquatic environment. Calculation of the exposure indices used supplementary information such as production volumes, from the IUCLID database [Heidorn et al., 1996] (see description in 15.3.3 below) where available. (IUCLID information was available for 318 of the 658 candidate substances, in particular IUCLID does not cover low production/import volume substances.) Substances were included on the monitoring-based lists only if they met specified criteria for their relevance at EU-level. Some substances were clustered (grouped) on the basis of being similar in nature and effect potential.

The final 32 recommended priority substances were selected from these ranked lists using a two stage process carried out on a substance by substance basis. Firstly the lists were screened and a subset of substances selected from each. Then recommendations were given for their inclusion in the final list of priority substances. Some substances were excluded from the final priority list because of limited data on exposure and use patterns.

The publication includes very detailed information on the exposure indices, effect indices and risk-based priority index used as well as the principles employed in selecting the final priority substances from the ranked lists. Details of information used for each substance are given, as are details of the monitoring data and supplementary information provided by Member States.

Additionally, the options considered for the statistical treatment and evaluation of the monitoring data are described in detail.

15.3.2 EU Ranking of Existing High Production Volume Chemicals: The 'EURAM' Method

The EU Risk Ranking Method, EURAM, is used to rank high production volume existing chemicals as part of setting priorities for in-depth chemical risk assessments. EURAM assigns ranking scores to chemicals according to relative concern for the environment and to people. It is described in [van Haelst & Hansen, 2000], [Hansen et al., 1999] and [Heidorn et al., 96] and builds on earlier work described in [Weiss et al., 1988].

EURAM was developed in support of Council Regulation 793/93/EEC [European Communities. Commission, 1993] which deals with evaluating and controlling the risks from existing high production chemicals. There are 100,195 EU existing chemicals, defined as those which were on the European market before September 1981 and are listed in the European Inventory of Existing Commercial Substances that are produced or imported in quantities exceeding 10 tonnes per year. The directive is concerned initially with the 2,474 [Haekst & Hansen, 2000] high production volume substances which have been imported or produced in quantities exceeding 1,000 tonnes per year. The directive sets out a framework for:

- data gathering;
- priority setting;
- risk assessment; and
- proposals for risk management.

Data is provided by producers and importers and stored in the International Uniform Chemical Information Database, IUCLID [Heidorn et al., 1996]. IUCLID is the basic tool for priority setting and is also used for the in-depth risk assessments. The priority setting procedure involves extracting the data from IUCLID, automated substance ranking using EURAM, and finally use of expert judgment to produce a proposed priority list. The procedure is described [Hansen, 1996] as `a relatively simple procedure, where a balance is sought between the time-saving and objective, but possibly inaccurate, results of automated methods and the time-consuming and subjective, but generally more accurate, results of expert judgment.' One criterion for selecting priority substances is lack of data (this is set in the directive). Each priority substance is assigned to a Member State Authority which carries out the risk assessment using guidance given in an EU `Technical Guidance Document'.

The EURAM ranking values representing concern for people are calculated using scores for human health effects and exposure. The scores for human health effects are largely based on substances' risk phrases which are considered together with information from IUCLID on tests for genetic toxicity, reproductive toxicity and repeated dose toxicity. The human health effects endpoints considered are acute toxicity, irritation, corrosivity, sensitisation, repeated dose toxicity, mutagenicity, carcinogenicity, and toxicity to reproduction. The scores for exposure take into account both emissions, based on tonnage produced or imported and use patterns, and distributions based on physicochemical properties for human exposure The exposure score reflects concern for workers and consumers. The third group of people of concern, those exposed through the environment, is not considered directly because this would be too complex for a ranking measure. However, concern for this group is partially captured in the environmental score.

Three main requirements were set for the development of EURAM, namely that it should be transparent, generally acceptable, and scientifically sound. The method was discussed and agreed over a 2 and a half year period including four technical meetings attended by scientific experts from the EU Member States, the European Free Trade Association, five industrial organizations, trade unions, and organizations such as the OECD. [Hansen et al., 1999] describes in detail how EURAM fulfils the criteria for a good chemical ranking scheme which were set out in [Swanson & Socha, 1999] and outlined in section 15.1.4 above.

16 APPENDIX 5: THE EU CLASSIFICATION SYSTEM FOR DANGEROUS SUBSTANCES AND COVERAGE OF DANGEROUS SUBSTANCES BY THE SEVESO II DIRECTIVE

This Appendix describes the EU classification system for dangerous substances and coverage of dangerous substances by the Seveso II Directive [European Communities. Commission, 1977 and 2003]. This is background information to the advice by the Critical Review Panel on a scope of substances for possible further AETLs development within the context of the risks of major accidents from chemical sites and in particular their regulation through the Seveso II Directive.

16.1 EU CLASSIFICATION OF DANGEROUS SUBSTANCES

In the EU, certain substances are classified according to Council Directive 67/548/EEC, the 'Dangerous Substances Directive', and its subsequent amendments. A number of substances have a harmonised classification that is legally binding in the EU. These are listed in Annex 1 of the Dangerous Substances Directive[33]. This is referred to as a substance's 'Annex 1 Classification'. The Directive is regularly amended[34] to include substances with newly agreed classifications. Additionally, these amendments may include modifications to the existing classification for a substance[35]. Substances which are not listed in Annex 1 must be self-classified by the supplier or Seveso II site operator according to the rules in Annex VI (Directive 2001/59/EC) to the Dangerous Substances Directive. Under these rules, substances may be assigned:

- *a classification*, the 'category of danger', which covers health effects such as Corrosive, Toxic, and Very Toxic, physicochemical effects such as Explosive, or environmental effects; together with
- *a 'risk phrase' or R-phrase* (such as Very Toxic by inhalation 'R26', and Flammable 'R10').

16.1.1 Classification of a Dangerous Substance as 'Toxic' or 'Very Toxic'

The classifications Toxic ('T') and Very Toxic ('T+') are specifically referred to in the Seveso II Directive and are therefore of particular relevance. They are based on the following descriptions.

- Toxic substances and preparations are those which in low quantities cause death or acute or chronic damage to health when inhaled, swallowed or absorbed via the skin.
- Very Toxic substances and preparations are those which in very low quantities cause death or acute or chronic damage to health when inhaled, swallowed or absorbed via the skin.

[33] The substances included in Annex 1 of the Dangerous Substances Directive and their classifications are available on the website of the European Classification Bureau: ecb.jrc.it/classification-labelling.

[34] The Dangerous Substances Directive has most recently been amended by the '27th ATP', where ATP refers to the Commission Directive 'Adaptations to Technical Progress' which updates or amends a Council Directive.

[35] The accuracy of Annex 1 classifications is discussed by [Ruden and Hansson, 2003]

The classifications include quantitative criteria. For example, the classification Very Toxic by inhalation ('T+ with R26') indicates that the substance has a 4 hour inhalation LC_{50} of < 0.5 mg/l (for gases and vapours).

We note that only substances which cause significant toxicity on single (acute) exposure are of relevance for a program of AETLs development. However, the Toxic classification covers toxicity resulting from both single and repeated long-term (chronic) exposure. The risk phrase R48 (in combination with R23, R24 and/or R25) denotes the property to cause toxicity on repeated exposure. The R-phases R23, R24, R25 and R39 indicate Toxic classifications relating to single exposure toxicity. Therefore, the ACUTEX Critical Review Panel is advising that substances classified as Toxic solely because of the assignment of R48 are out of scope for AETLs development.

The Toxic and Very Toxic classifications are only two of the health related classifications that may be assigned to a dangerous substance. For example, a dangerous substance may be classified as Harmful, Corrosive or Irritant but not have a sufficiently high LC_{50} to be classed as Toxic or Very Toxic.

16.2 DANGEROUS SUBSTANCES COVERED BY THE SEVESO II DIRECTIVE AND THE ROLE OF CLASSIFICATION

Installations covered by the Seveso II Directive may present risks to people or the environment. Substances are included under the directive either:

- as a '*Named Substance' or group of substances* (listed in Annex 1, Part 1 of the Seveso II Directive); or
- as being classified under one or more *generic 'Categories of Substances and Preparations'* (listed in Annex 1, Part 2 of the Seveso II Directive).

For both the Named Substances, and the generic categories, the Directive specifies two sets of 'Qualifying Quantities' in tonnes. These are threshold quantities of substances used to define which establishments fall within the scope of the Directive, either as 'lower-tier' or 'top-tier' sites. The qualifying quantities apply to the amount of a dangerous substance which is either actually present, anticipated, or which may be generated in an incident. Table 16.1 gives examples of some Qualifying Quantities.

16.2.1 The Seveso II Named Substances or Groups of Substances

There are 29 Named Substances (or groups of substances) in addition to the Named Carcinogens which comprise a further 17 substances (or groups of substances). The Named Carcinogens are thought to pose a risk of carcinogenicity following a single exposure, and are often termed 'one-shot carcinogens'.

Table 16.1: Examples of Qualifying Quantities for Dangerous Substances Specified in the Seveso II Directive

Dangerous Substances	Qualifying Quantity (tonnes)	
	Lower-Tier Sites (Articles 6 and 7)	Top-Tier Sites (Article 9)
Phosgene (A Named Substance which is classified as Very Toxic)	0.3	0.75
Named Carcinogens	0.5	2
Very Toxic Generic Substances	5	20
Chlorine (A Named Substance which is classified as Toxic)	10	25
Toxic Generic Substances	50	200

16.2.2 The Seveso II Generic Categories of Substances and Preparations

The Seveso II Directive lists 10 generic categories of dangerous substances and preparations. Of these, two are relevant to human health in relation to toxicity while the remainder deal with harm to the environment, or with explosive, flammable, oxidising, or water-reactive hazardous properties. The two relevant categories are:

- Category 1 'Very Toxic'; and
- Category 2 'Toxic'.

We do not know how many substances and preparations meeting these classifications are present, anticipated, or may be generated at Seveso II sites across the EU.

16.2.3 Toxic and Very Toxic Classifications Linked to Inhalation and Relevance to the Recommended Scope of Substances in Relation to Chemical Site

The ACUTEX project is developing an AETL methodology for inhalation by people of toxic substances. However, if a substance has Annex 1 Classification as Toxic or Very Toxic, but does not have an inhalation risk phrase, it is still within the recommended scope. This is because the lack of an inhalation risk phrase does not necessarily mean that a substance is not Toxic or Very Toxic by the inhalation route. For example, it may simply reflect a limited availability of acute inhalation data for the substance. Oxybenzene (phenol) is an example of a substance in the preliminary list of 21 case studies for AETLs development which has no inhalation risk phrase. It has Annex 1 Classification Toxic T; R24, R25, R34 (toxic in contact with skin or if swallowed, and causes burns) and is within the recommended scope.

16.3 MODIFICATIONS TO HAZARDOUS SUBSTANCES COVERED IN THE IMPLEMENTATION OF THE SEVESO II DIRECTIVE BY INDIVIDUAL MEMBER STATES

So far as we understand, in implementing the Seveso II Directive, some Member States have:

- included additional substances; or
- broadened the hazardous properties of substances which must be considered in terms of off-site risk; or
- reduced the Qualifying Quantities specified in the Directive.

We have no details of the extent to which this has been done.

The Critical Review Panel took this into account in making their recommended scope of substances. Therefore the scope encompasses some substances identified by Competent Authorities as being of particular interest in terms of off-site risk at chemical sites, but which are not covered by the Seveso Directive.

We note that the Critical Review Panel advised against including substances in the scope which have the classification of sensitisation by inhalation (indicated by the risk phrase R42). These substances are respiratory sensitisers and are of interest to some Competent Authorities because they have the potential to cause adverse reactions in sensitised persons at very low exposure levels. The Critical Review Panel's advice was given because more than one exposure to a respiratory sensitiser is required to induce a sensitisation reaction.

Additionally, the Critical Review decided against taking into account the reduced Qualifying Quantities which some Member States have used when implementing the Seveso II Directive. Some Member States had suggested taking this into account.

17 APPENDIX 6: THE LACOURSIERE RANKING FACTOR BASED ON SUBSTANCE INHERENT PROPERTIES

Canadian regulatory work [Lacoursiere, 2002] in support of defining threshold quantities in respect of potential releases of toxic substances from chemical plant uses the following ranking factor based on substance inherent properties.

IDLH/V where:

- IDLH = Immediately Dangerous to Life and Health toxicity level . [Ludwig et al., 1994];
- V = 1 for substances that are gases under ambient conditions;
- V = $(1.6 \times MW^{0.67}) / (T+273)$ for substances that are liquids under ambient conditions;
- MW = molecular weight; and
- T = boiling temperature in ^{o}C.

18 APPENDIX 7: DETAILS OF CALCULATIONS FOR HAZARD MEASURES FOR THREE EXAMPLE FLUIDS

Gas dispersion from a catastrophic release to the $4hLC_{50}$ concentration was modelled for four substances selected from the substances nominated by Competent Authorities in their lists of '10 Substances of Interest'. These are chlorine, ammonia, and sulphur dioxide which are all classified as Toxic, and monomethylamine which is in scope as a misclassified Toxic. This was done for two release quantities:

- a 20 te reference quantity, and
- the Seveso II top-tier (Article 9) Qualifying Quantity.

The source terms for each release were calculated using the in-house HSE model IRATE3. This model was used to generate the aerosol fraction, the mass of air entrained into the initial cloud, and the final equilibrium temperature on release. The outputs from the source term model were used as part of the input to the DENZ [Fryer & Kaiser, 1979] gas dispersion model.

We have done this in order to illustrate the hazard measures. As we discussed in section 6.3.1, other models could be used. However, because the outcome is to be used for *ranking* purposes, rather than to give absolute plume areas and extent, we consider that the specific models used are not an issue, although the use of consistent models and assumptions for the different substances is essential.

Below we give a brief description of the inputs and outputs for these two models, followed by the values for each of the releases we modelled.

18.1 INPUTS AND OUTPUTS FOR CATASTROPHIC RELEASE MODELLING

Here we give a brief description of the inputs used to model the source terms and dispersion for a catastrophic release and the outputs generated by the models. We explain the choice of the values that remain constant for all of the releases modelled. In all cases it was assumed that the release occurred from pressurized storage at ambient temperature.

18.1.1 IRATE3 Source Term Inputs

Quantity Released (kg)
Two quantities were modelled for each substance, the reference quantity of 20 tonnes (20000 kg), and the Seveso II top-tier Qualifying Quantity, namely: 200 tonnes (200000 kg) for the generic Toxic substances, ammonia, and sulphur dioxide; and 25 tonnes (25000 kg) for the Named Substance chlorine.

Air Temperature = 278 °K
Assumed standard night temperature consistent with use of F2 weather conditions (see gas dispersion inputs).

Stagnation Temperature = 288 °K
Assumed standard daytime temperature. It is assumed that the cooling effect of the standard night temperature will have little effect on the substance temperature.

18.1.2 IRATE3 Source Term Outputs

Aerosol Fraction
The amount of the liquid that is entrained into the cloud as an aerosol after the initial flash fraction has evaporated from a release of a pressure liquefied gas. The aerosol fraction is equal to 1 minus the flash fraction, as it is assumed that the remaining quantity of the substance is entrained after flashing.

Mass of Air Entrained (kg)
The amount of air entrained into the substance cloud upon release, which dilutes the gas prior to dispersion.

Final Equilibrium Temperature (°K)
It is assumed that the gas cools from the stagnation temperature as it depressurises and expands. The final equilibrium temperature is the temperature of the cloud as the dispersion phase begins.

18.1.3 DENZ Gas Dispersion Inputs

Release Quantity (te)
Either the reference quantity of 20 tonnes, or the top-tier Qualifying Quantity for the substance.

Release Temperature (°K)
Equivalent to the source term final equilibrium temperature.

F2 Weather Conditions: Pasquill Weather Stability Category = F; Wind speed = 2 ms^{-1}
The use of the F category, representative of stable atmospheric conditions, and a low wind speed produces little turbulence to mix the contaminant substance with air so that the cloud dilutes less rapidly than for less stable atmospheric conditions, or higher wind speeds. The low wind speed also allows the cloud to spread laterally (slump) under its own weight rather than being driven by the wind, as would be the case for higher wind speeds. The cloud will travel further for these conditions, both downwind and crosswind, before diluting beneath the concentration of interest, than for when less stable atmospheric conditions or higher wind speeds are modelled. Consequently, it is assumed that F2 conditions will provide 'worst-case' dispersion plumes when assessing the plume area from a release.

Air Temperature = 278 °K
Assumed standard night temperature consistent with use of F2 weather conditions.

Ground Roughness = 0.3 m
Assumed representative of housing/urban area.

Concentration of Interest (ppm)
The 4h LC_{50} value for the substance has been used as the concentration of interest. The plume footprint to the 4h LC_{50} concentration is modelled.

Aspect ratio = 1
The cloud is modelled as a cylinder. The aspect ratio is the ratio of the height of the source term cylinder to its radius.

Dilution
Taken from source term model. The ratio of the mass of air entrained into the cloud on release to the quantity of substance released.

Aerosol Fraction
Obtained from source term model.

18.1.4 DENZ Gas Dispersion Outputs

Axial Distance (m)
Maximum downwind distance on centreline axis.

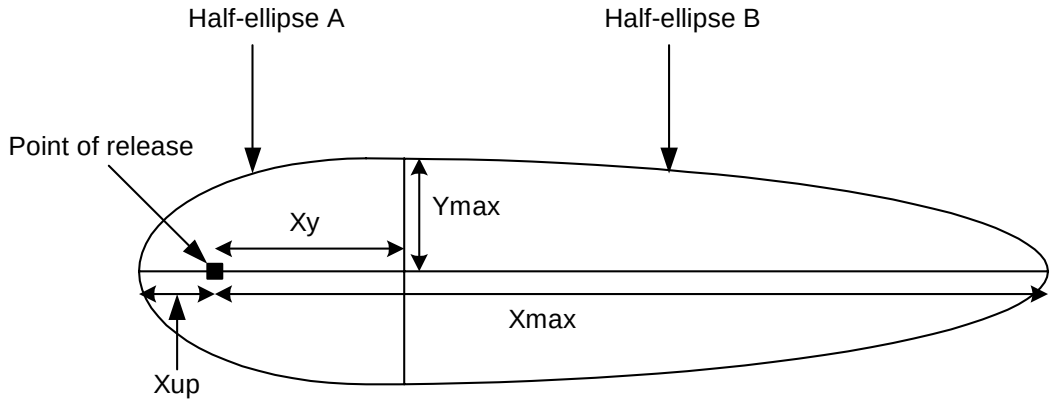
Upwind Axial (m)
Maximum upwind spread on centreline axis.

Maximum Half Width (m)
Maximum crosswind extent of cloud.

Axial Distance to Max Half-Width (m)
The downwind distance on the centreline axis at which the maximum crosswind extent is reached.

Plume Area (km^2)
Calculated from the axial and crosswind distances. The plume is treated as two half-ellipses, as shown in figure 17.1.

Figure 17.1: Plume as two half-ellipses



Xmax = Axial distance (m)
Xup = Upwind axial (m)
Ymax = Maximum half-width (m)
Xy = Axial distance to max half-width (m)

In figure 17.1, half-ellipse A has:
Semi-major axis = Xup + Xy;
Semi-minor axis = Ymax.

Half-ellipse B has:
Semi-major axis = Xmax – Xy
Semi-minor axis = Ymax

18.2 INPUTS AND OUTPUTS FOR THE RELEASES MODELLED

18.2.1 Chlorine – 20 te Reference Quantity

Table 17.1 lists the source term inputs and outputs, and Table 17.2 lists the gas dispersion inputs and outputs.

Table 17.1: Source Terms for Catastrophic Release of 20 te of Chlorine

Source term inputs		***Source term outputs***	
Mass released (kg)	20000	Aerosol fraction	0.854
Stagnation temperature (°K)	288	Mass of air entrained (kg)	81900
Air temperature (°K)	278	Final equilibrium temperature (°K)	224.3

Table 17.2: Gas Dispersion for Catastrophic Release of 20 te of Chlorine

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	20	Axial distance (m)	17704
Release temperature (°K)	224.3	Upwind axial (m)	-98
Air temperature (°K)	278	Maximum half-width (m)	755
Pasquill stability category	F	Axial distance to max half-width (m)	1500
Wind speed (ms^{-1})	2.0	Plume area (km^2)	21.1
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.854		
Dilution	4.095		
Concentration of interest (ppm)	44.91		

18.2.2 Chlorine – Top-tier Qualifying Quantity, 25 te

Table 17.3 lists the source term inputs and outputs, and table 17.4 lists the gas dispersion inputs and outputs.

Table 17.3: Source Terms for Catastrophic Release of 25 te of Chlorine

Source term inputs		***Source Term Outputs***	
Mass released (kg)	25000	Aerosol fraction	0.854
Stagnation temperature (°K)	288	Mass of air entrained (kg)	95000
Air temperature (°K)	278	Final equilibrium temperature (°K)	220.9

Table 17.4: Gas Dispersion for Catastrophic Release of 25 te of Chlorine

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	25	Axial distance (m)	20379
Release temperature (°K)	220.9	Upwind axial (m)	-108
Air temperature (°K)	278	Maximum half-width (m)	842
Pasquill stability category	F	Axial distance to max half-width (m)	1500
Wind speed (ms^{-1})	2.0	Plume area (km^2)	27.1
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.854		
Dilution	3.8		
Concentration of interest (ppm)	44.91		

18.2.3 Ammonia – 20 te Reference Quantity

Table 17.5 lists the source term inputs and outputs, and table 17.6 lists the gas dispersion inputs and outputs.

Table 17.5: Source Terms for Catastrophic Release of 20 te of Ammonia

Source term inputs		***Source term outputs***	
Mass released (kg)	20000	Aerosol fraction	0.848
Stagnation temperature (°K)	288	Mass of air entrained (kg)	218000
Air temperature (°K)	278	Final equilibrium temperature (°K)	204.6

Table 17.6: Gas Dispersion for Catastrophic Release of 20 te of Ammonia

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	20	Axial distance (m)	1470
Release temperature (°K)	204.6	Upwind axial (m)	-138
Air temperature (°K)	278	Maximum half-width (m)	418
Pasquill stability category	F	Axial distance to max half-width (m)	750
Wind speed (ms^{-1})	2.0	Plume area (km^2)	1.06
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.848		
Dilution	10.9		
Concentration of interest (ppm)	2072		

18.2.4 Ammonia – Top-tier Qualifying Quantity, 200 te

Table 17.7 lists the source term inputs and outputs, and table 17.8 lists the gas dispersion inputs and outputs.

Table 17.7: Source Terms for Catastrophic Release of 200 te of Ammonia

Source term inputs		***Source term outputs***	
Mass released (kg)	200000	Aerosol fraction	0.848
Stagnation temperature (°K)	288	Mass of air entrained (kg)	1010000
Air temperature (°K)	278	Final equilibrium temperature (°K)	207.7

Table 17.8: Gas Dispersion for Catastrophic Release of 200 te of Ammonia

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	200	Axial distance (m)	3691
Release temperature (°K)	207.7	Upwind axial (m)	-392
Air temperature (°K)	278	Maximum half-width (m)	1036
Pasquill stability category	F	Axial distance to max half-width (m)	2000
Wind speed (ms^{-1})	2.0	Plume area (km^2)	6.64
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.848		
Dilution	5.05		
Concentration of interest (ppm)	2072		

18.2.5 Sulphur dioxide – 20 te Reference Quantity

Table 17.9 lists the source term inputs and outputs, and table 17.10 lists the gas dispersion inputs and outputs.

Table 17.9: Source Terms for Catastrophic Release of 20 te of Sulphur Dioxide

Source term inputs		***Source term outputs***	
Mass released (kg)	20000	Aerosol fraction	0.917
Stagnation temperature (°K)	288	Mass of air entrained (kg)	60404
Air temperature (°K)	278	Final equilibrium temperature (°K)	220.0

Table 17.10: Gas Dispersion for Catastrophic Release of 20 te of Sulphur Dioxide

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	20	Axial distance (m)	1753
Release temperature (°K)	220.0	Upwind axial (m)	-99
Air temperature (°K)	278	Maximum half-width (m)	384
Pasquill stability category	F	Axial distance to max half-width (m)	750
Wind speed (ms^{-1})	2.0	Plume area (km^2)	1.12
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.917		
Dilution	3.02		
Concentration of interest (ppm)	557		

18.2.6 Sulphur dioxide – Top-tier Qualifying Quantity, 200 te

Table 17.11 lists the source term inputs and outputs, and table 17.12 lists the gas dispersion inputs and outputs.

Table 17.11: Source Terms for Catastrophic Release of 200 te of Sulphur Dioxide

Source term inputs		***Source term outputs***	
Mass released (kg)	200000	Aerosol fraction	0.917
Stagnation temperature (°K)	288	Mass of air entrained (kg)	281000
Air temperature (°K)	278	Final equilibrium temperature (°K)	223.5

Table 17.12: Gas Dispersion for Catastrophic Release of 200 te of Sulphur Dioxide

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	200	Axial distance (m)	4302
Release temperature (°K)	223.5	Upwind axial (m)	-289
Air temperature (°K)	278	Maximum half-width (m)	958
Pasquill stability category	F	Axial distance to max half-width (m)	2000
Wind speed (ms^{-1})	2.0	Plume area (km^2)	6.91
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.917		
Dilution	1.405		
Concentration of interest (ppm)	557		

18.2.7 Monomethylamine – 20 te Reference Quantity

Table 17.13 lists the source term inputs and outputs, and table 17.14 lists the gas dispersion inputs and outputs.

Table 17.13: Source Terms for Catastrophic Release of 20 te of Monomethylamine

Source term inputs		***Source term outputs***	
Mass released (kg)	20000	Aerosol fraction	0.91
Stagnation temperature (°K)	288	Mass of air entrained (kg)	102000
Air temperature (°K)	278	Final equilibrium temperature (°K)	224.7

Table 17.14: Gas Dispersion for Catastrophic Release of 20 te of Monomethylamine

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	20	Axial distance (m)	1630
Release temperature (°K)	224.7	Upwind axial (m)	-124
Air temperature (°K)	278	Maximum half-width (m)	345
Pasquill stability category	F	Axial distance to max half-width (m)	750
Wind speed (ms^{-1})	2.0	Plume area (km^2)	0.951
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.91		
Dilution	5.1		
Concentration of interest (ppm)	947		

18.2.8 Monomethylamine – Top-tier Qualifying Quantity, 200 te

Table 17.15 lists the source term inputs and outputs, and table 17.16 lists the gas dispersion inputs and outputs.

Table 17.15: Source Terms for Catastrophic Release of 200 te of Monomethylamine

Source term inputs		***Source term outputs***	
Mass released (kg)	200000	Aerosol fraction	0.91
Stagnation temperature (°K)	288	Mass of air entrained (kg)	474000
Air temperature (°K)	278	Final equilibrium temperature (°K)	229.1

Table 17.16: Gas Dispersion for Catastrophic Release of 200 te of Monomethylamine

Gas dispersion inputs		***Gas dispersion outputs***	
Release quantity (te)	200	Axial distance (m)	4283
Release temperature (°K)	229.1	Upwind axial (m)	-400
Air temperature (°K)	278	Maximum half-width (m)	856
Pasquill stability category	F	Axial distance to max half-width (m)	2000
Wind speed (ms^{-1})	2.0	Plume area (km^2)	6.30
Ground roughness (m)	0.3		
Aspect ratio	1.0		
Aerosol fraction	0.91		
Dilution	2.37		
Concentration of interest (ppm)	947		

MAIL ORDER
HSE priced and free
publications are
available from:
HSE Books
PO Box 1999
Sudbury
Suffolk CO10 2WA
Tel: 01787 881165
Fax: 01787 313995
Website: www.hsebooks.co.uk

RETAIL
HSE priced publications
are available from booksellers

HEALTH AND SAFETY INFORMATION
HSE Infoline
Tel: 0845 345 0055
Fax: 0845 408 9566
Textphone: 0845 408 9577
e-mail: hse.infoline@natbrit.com
or write to:
HSE Information Services
Caerphilly Business Park
Caerphilly CF83 3GG

HSE website: www.hse.gov.uk

RR 426