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Review and Comments on the Model ACE

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QA Sheet

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1 Acronyms and Definitions

Acronym	Definition
ACE	Airborne Concentration Estimate source term model originally developed for HSE by WS Atkins
ascii	Character encoding based on English alphabet (American Standard Code for International Exchange)
BLEVE	Boiling Liquid Expanding Vapour Explosion
CFD	Computational Fluid Dynamics
COM	Component Object Model – a Microsoft Windows technology for communication between software components
DRIFT	Dispersion model developed for HSE by ESR Technology
GASP	Pool spreading and evaporation model developed for HSE by AEA Technology (now ESR Technology)
HSE	Health and Safety Executive
HSL	Health and Safety Laboratory
LPG	Liquefied Petroleum Gas
IRATE	Instantaneous release source model previously used by HSE
SPI	Substance Property Information - file format used by certain HSE models to access data for substance property correlations

2 Introduction

1. Airborne Concentration Estimate (ACE) is a simple source term model aimed at estimating source conditions arising from catastrophic failure of vessels containing pressure liquefied gas. The output from ACE is intended for input to a subsequent gas dispersion model such as DRIFT.

2. As part of the work package aimed at characterising source terms suitable for DRIFT Version 3, GT Science and Software has been asked to undertake a quick review and to provide comments on the suitability of using the ACE model, in particular when using ACE together with DRIFT. This report is a record of the findings of this review.

3. The Health and Safety Laboratory (HSL) has recently modified ACE to access substance properties data from HSE's SPI (Substance Property Information) files, rather than using data built directly into ACE. This, in principle, gives ACE access to a wider range of substances. A pertinent question is therefore the extent to which ACE is dependent on particular substance properties that might limit its generalisation to the wider range of SPI substances. We consider this when reviewing the model.

4. In parallel with this review, HSL has undertaken DRIFT dispersion sensitivity runs using ACE [1]. HSL has further investigated the validity of the ACE model by comparing ACE predictions with published experimental data [2].

3 Background

5. Catastrophic failure of a pressure vessel containing pressure liquefied gas will result in the rapid, near instantaneous release of the vessel contents. A fraction of the released liquid will rapidly vaporise (flash) to vapour. The remaining liquid may, depending upon the release conditions, break-up and form an airborne aerosol cloud and/or be deposited on surrounding surfaces and the ground (liquid rainout). Any vapour present in the space above the liquid in the vessel will also rapidly expand on loss of containment. The energy associated with the initial release drives a rapid initial expansion of the cloud and its initial mixing with the surrounding ambient air.

6. Experimental studies, e.g. [3], usually at small scale, have aided the understanding of the behaviour of catastrophic flashing releases. However, mathematical modelling of the complex processes that occur is very challenging.

7. In some circumstances, e.g. for substances which are toxic at low concentrations, hazard ranges may not be particularly sensitive to the dilution associated with initial catastrophic failure and the associated cloud expansion. In others, e.g. flammable substances, the cloud may dilute to below flammable concentration during the initial expansion phase. Ignoring the initial expansion phase may therefore be regarded as a reasonable approximation for very toxic substances which are little influenced by dilution at the source, but cautious, possibly overly so, for flammable substances which are greatly influenced by dilution at the source.

8. DRIFT's instantaneous cloud model allows for buoyancy and aerosol effects and, as of Version 3, can also model flashing from an initially superheated liquid state. However, DRIFT's instantaneous model does not including modelling of the effect of the initial expansion driven dilution or liquid rainout. Therefore, there is a requirement to consider the appropriate specification of these when using DRIFT for modelling releases from catastrophic vessel failure.

9. ACE was originally developed for HSE by WS Atkins in the late 1990s [4]. [5] describes enhancements and revisions to the model. HSE holds source code to the ACE model, allowing checks on the computer implementation, and if necessary allowing changes to be made. An addendum to this report (see Section 6) details subsequent changes to the ACE model.

4 ACE Model

4.1 Modelling Regimes

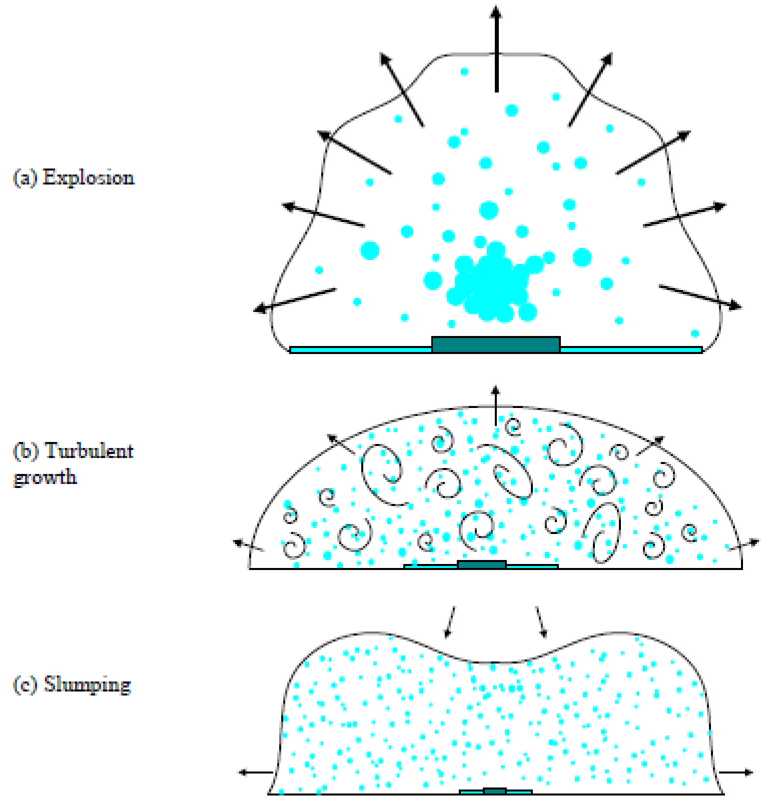

Figure 4-1 Modelling regimes adopted by ACE from [5]

10. For the convenience of modelling, the evolution of the cloud is considered in the following distinct regimes (see Figure 4-1):

    a) Rapid expansion (flash depressurisation)
    b) Slower expansion (turbulent growth)
    c) Slumping/advection (dense gas dispersion)

11. ACE models the first two of these regimes and estimates the point of transition to the third, from which a conventional gas dispersion model may be run.

4.2 Rapid Expansion Phase Sub-Model

4.2.1 Model Equations

12. For the rapid expansion phase, ACE adopts the model of [6], albeit with some adjusted parameter values which are detailed below.

13. We note that the following:

    a. The Shield model is mainly intended for prediction of BLEVE fireballs.
    b. The expansion model is based on observations from videos of large scale LPG BLEVE experiments at Spadeadam [7].

14. Initial expansion growth of the cloud radius *R* is modelled as

$$R = U_0 t_p \left[1 - \exp\left(-\frac{t}{t_p}\right)\right] \qquad (4\text{-}1)$$

with

$$U_0 t_p = NL$$

$$L^3 = \alpha\, \beta\, M\, / \rho_{v0}$$

15. U_0 is a characteristic initial velocity; t_p is a characteristic expansion timescale; *N* is a parameter discussed further below; *L* is a length scale based on the volume of vapour present after flash depressurisation; *α* is the initial liquid mass fraction before vessel rupture; *β* is the mass fraction of vapour flashed from the liquid; *M* is the storage mass; ρ_{v0} is the saturated vapour density at atmospheric pressure.

16. Shield interprets *N* as being the number of eddies, which he assumes, based on his observation of the videos, remains constant as the cloud expands. [4] studied videos of the same LPG BLEVE trials but were unable to corroborate this observation of Shield. With this assumption, Shield relates the velocity scale U_0 to the turbulent velocity scale u_L.

$$U_0 = N^2 u_L \qquad (4\text{-}2)$$

17. Shield further assumes a balance between the initial turbulent kinetic energy and the work done in expanding against the atmosphere to derive an expression relating *N* to the turbulent velocity scale u_L

$$N = \left[\left(\frac{P_0}{G_1 \rho_a u_L^2}\right) - \left(\frac{\rho_{v0}}{G_1 \alpha \beta \rho_a}\right) + \left(\frac{1}{G_1}\right) + \frac{(1-\beta)\rho_{v0}}{G_1 \beta \rho_{L0}}\right] \qquad (4\text{-}3)$$

G_1 is a geometric factor (=4π/3 for a spherical cloud)

ρ_{L0} is the saturated liquid density

ρ_a is the air density

P_0 is ambient air pressure

18. Shield closes the equation set for the initial cloud growth by setting

$$u_L = 39.85 \left(\frac{\rho_a^2}{\rho_{vT}\rho_{v0}}\right)^{\frac{1}{9}} (\alpha\beta)^{1/9} \text{ [m/s]} \qquad (4\text{-}4)$$

which he claims is the best fit to the large scale data of [7] as well as smaller scale data including that of [8]. The experiments involve releases of butane, propane and propylene. In all of the experiments fitted the resulting value of *N* is stated as being between 2.6 and 2.7.

19. [4] questions the justification for Shield's assumed balance between turbulent kinetic energy and work done against the atmosphere. In the version of ACE described in [4] *N* is set to the mean value of Shield's range, i.e. 2.65. In the revised ACE described in [5] *N* is set to a smaller value of 2.35 and the turbulence velocity u_L is a user input with a suggested default value of 10 m/s, as compared with 30-35 m/s given by equation (4-4).

20. The volume at the end of the rapid expansion phase is N^3 times the volume of vapour flashed from the liquid. Therefore the change in going from *N* = 2.65 to *N* = 2.35 corresponds to a 30% decrease in volume or approximately 10% decrease in cloud radius. These changes are quite small and explain why the radius at the end of the rapid expansion phase is little affected by the changes. The timescale t_p for the radial expansion is however much more sensitive, changing by approximately a factor of 3 between the original and revised ACE versions - due mainly to the change in u_L. [5] do not mention this, perhaps assuming that given its short duration, the time scale of the initial rapid expansion phase is not particularly important if the dilution as implied by the cloud radius remains very similar (within 30%). However, this reduction in the turbulence velocity scale to 10 m/s could mean that the timescale for the rapid growth is no longer in accord with expansion timescale of the large scale BLEVE tests from which Shield derived the values in equation (4-4).

21. In the Shield model, the fireball expansion time (after ignition) is dependent on the turbulence velocity scale, u'. Reducing the turbulence velocity in the cloud (as in the revised ACE) may lead to the results for fireball expansion no longer being well predicted. However, this may not be important since other factors also influence the fireball duration and ACE is not intended to be used for fireball modelling.

4.2.2 Validation of the Rapid Expansion Sub-Model

22. [4] present validation of the rapid expansion phase model in terms of comparison of the final radius after rapid expansion with experimental observations and with CFD predictions.

23. Comparisons of the predicted radius at the end of the rapid expansion phase are made with the observed radius in the small scale propylene experiments of [8] and with the stated aerosol cloud radius from the small scale Refrigerant 11 releases of [9], although it is not clear that this latter cloud size relates entirely to the rapid expansion phase. Good agreement is claimed.

24. [4] also claim that the predictions are consistent with the experimental observations of [10] and [11], but it is unclear what they mean by this since they also state that in neither

of these cases are there measurements that can be compared directly with the radii predicted by the rapid expansion sub-model.

25. [4] assumes, since the Shield model was derived from and fitted to the Spadeadam LPG BLEVE tests, that it is reasonable that the model should reproduce the results from these large-scale experiments fairly well. However, they also note that it was not possible to derive the cloud volumes from the videos of these experiments and hence it was not possible to confirm independently the predictions of the model.

26. [4] also compares predictions with the radius from the medium scale (422 kg) propane experiments of [12] which involved rapid loss of emptying through an orifice in a tank. The radius predicted at the end of the expansion phase in ACE is compared with the time dependent growth observed in [12], reproduced in Figure 4-2 below. [4] considers that, given the differences between model and experiment, the ACE prediction is consistent. Although somewhat subjective, we concur with this statement in as much as the ACE predicted radius is consistent with the observed radius after some slowing down from a rapid expansion, but is less than the radius in the slower expansion phase.

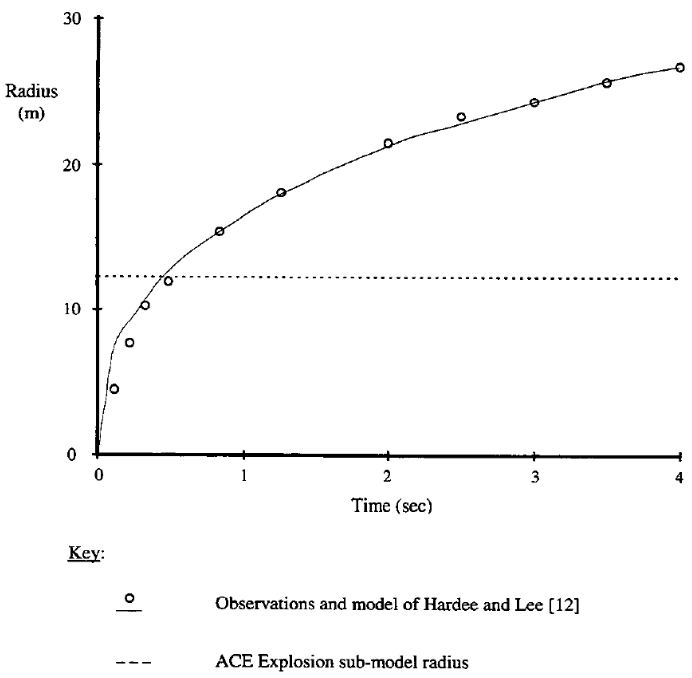

Figure 4-2 Comparison of ACE rapid expansion sub-model final radius with 422 kg propane release: taken from [4]

27. The revisions to ACE reported in [5] result in little change (typically ~10% reduction) to the predicted radius of the cloud at the end of the rapid expansion phase, although as already mentioned there is an implication for the time over which this occurs. Unfortunately only the radius, rather than the time at which this occurs (or the expansion velocity) are compared with experimental data.

4.2.3 Comments on the Rapid Expansion Sub-Model

28. It is easy to question many of the assumptions made in deriving the Shield model equations, for example:

    1. The assumption that the number of eddies remains constant whilst the cloud expands.

    2. The assumption of constant eddy viscosity and diffusivity.

    3. The conversion between mean radial expansion and turbulent velocity.

    4. The energy balance on the expanding cloud.

29. However, in our view, given the empirical nature of the model, and its fitting to/derivation from both large scale and small scale data, then perhaps these aspects are less important than they would be otherwise. We recognise that any simple model will need to make simplifying assumptions which *a priori* might not have a strong basis, which can only be justified in the light of validation against data. It is encouraging that the Shield model appears capable of describing both large and small scale experiments for a range of fluids (propane, butane and propylene).

30. It is reassuring that the end radius of the rapid expansion phase is rather insensitive to uncertain model parameters. In fact one could argue that a much simpler model is possible by simply relating the cloud volume to the flashed vapour volume. Uncertainty in the turbulence velocity scale leads to uncertainty in the timescale for the initial rapid growth, but perhaps more importantly uncertainty for the subsequent slower turbulence driven growth phase of the model.

31. Given the immense difficulties of modelling such flashing two-phase releases using CFD, the results from the CFD modelling reported in [4] are regarded at best as being uncertain. Hence reliance on CFD quantitative results would ideally be kept to a minimum.

32. A justifiable view of the change in the revised ACE is that an extra degree of caution to the subsequent turbulent growth has been introduced by assuming a lower turbulence velocity scale than in the Shield model and that such caution is appropriate given the modelling uncertainties.

33. Comparisons of the time-dependent growth with suitable experimental measurements, e.g. [3] or models fitted to experimental data, e.g. the spray expansion model of [8], might be useful to reduce the uncertainty in the expansion model. Subsequent ACE validation reported in [2] includes such comparisons.

4.3 Turbulent Growth Phase Sub-Model

34. Following the initial rapid expansion phase, ACE models a slower turbulent driven growth phase. In this phase the cloud is assumed to grow by turbulence generated by the initial expansion growth. Gravity slumping is neglected in this turbulent growth phase which is assumed to terminate when the characteristic velocity scale for gravity slumping exceeds the turbulence velocity scale in the cloud. At this gravity slumping transition the

characteristics of the cloud (size, dilution, etc.) form the basis of the source term for the subsequent dispersion model.

4.3.1 Dilution and Spreading

35. ACE uses a k-ε model applied to the bulk cloud with the empirical parameters of the model fitted to CFD model predictions.

$$\frac{dk}{dt} = -\frac{bk^{\frac{3}{2}}}{r} - \epsilon \tag{4-5}$$

$$\frac{dr}{dt} = \frac{bk^{\frac{1}{2}}}{3} \tag{4-6}$$

$$\frac{d\epsilon}{dt} = -C_{2\epsilon}\frac{\epsilon^2}{k} \tag{4-7}$$

where

k	is the turbulent kinetic energy per unit mass (m^2s^{-2})
r	is the cloud radius (m)
ϵ	is the rate of turbulent dissipation (m^2s^{-3})
b	is a dimensionless constant
$C_{2\epsilon}$	is a dimensionless constant

36. The initial conditions are taken from the quantities predicted at the end of the rapid expansion sub-model:

$$k_0 = \frac{3\,u_L^2}{2} \tag{4-8}$$

$$r_0 = \left(\frac{3\,V_c}{n\,\pi}\right)^{1/3} \tag{4-9}$$

$$\epsilon_0 = \frac{C_\mu^{3/4} k_0^{3/2}}{L} \tag{4-10}$$

where

n	is 2 for a hemispherical cloud and 4 for a spherical cloud
V_c	is the volume of the cloud at the end of the rapid expansion phase
C_μ	is a dimensionless constant

37. The values of b = 1.0 and $C_{2\epsilon}$ = 2.1 adopted by ACE are obtained by fitting cloud growth results to CFD predictions of a hemispherical 30 te chlorine release. C_{μ} is set to a value of 0.09 as indicated in Appendix 6 of [4].

38. The above equations model the turbulent growth of the cloud, allowing for turbulence decay via dilution and turbulent dissipation. As shown in Appendix 6 of [5] this approach has parallels with a bulk (integral) modelling approach with the cloud radius growing at a rate directly proportional to the turbulent velocity scale. Such a relation between the cloud radius and turbulent velocity scale seems reasonable and is expected on dimensional grounds. The validity of equation (4-7) describing the dissipation of turbulence is less clear. Although widely used as a grid-scale turbulence model in CFD analysis, the validity of a homogeneous k-ε model applied to larger scale bulk cloud variables is quite a strong assumption, the validity of which is uncertain.

39. We note that the Boussinesq assumption is made whereby the variation of cloud density is neglected in the turbulent kinetic energy equation. This is a common assumption, but is questionable where the cloud density is significantly greater than ambient air density.

40. In our view this simple turbulent growth model is best regarded as being an empirical model which should be validated by comparison with suitable experimental data. Ideally, rather than being determined from comparison with uncertain CFD predictions, the parameters of the model should also be derived from fitting to experimental data. However, we recognise that there may not be sufficient experimental data to determine all the model parameters in this way and reliance may have to be made on CFD predictions for some parameters. This is justified if validation of the model indicates acceptable agreement of model predictions with experimental data. The reader is referred to [2] for the results of validation of ACE against such data.

4.3.2 Airborne Fraction

41. Airborne fraction is used as a basis for determining the initial aerosol content of the cloud, optionally the model can assume complete deposition (rainout) of aerosol or complete vaporisation of aerosol.

42. Airborne fraction is based on a plot of experimental results on airborne fraction as aerosol as a function of flash fraction (see Figure 4-3). There is much scatter in the data. In the original ACE a single linear fit was put through the data. In the revised ACE two curves are included representing approximately the upper and lower parts of the data. This seems a reasonable approach to representing the spread – although attributing one curve with omni-directional and the other with downward directed releases (as is done in the revised ACE) is open to question.

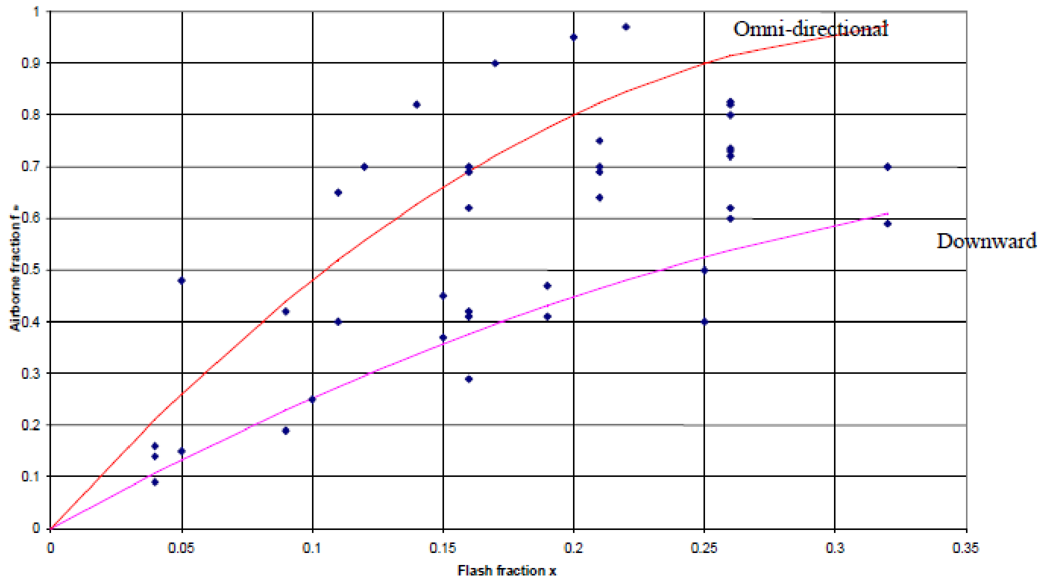

Figure 4-3 Airborne Fraction correlations in ACE from [5]

43. The effect of vessel fill fraction on airborne fraction is ignored in ACE. The justification given by [5] is based on the observation that the effect of fill fraction is less important at higher storage pressures in the results of [13]. [5] considers the saturation pressure of stored pressure liquefied substances as being generally greater than 5 bara.

44. In our opinion, correlation of airborne fraction with flash fraction is a reasonable approximation for simple modelling.

4.3.3 Droplet Modelling

45. ACE includes a liquid droplet model for the aerosol. The liquid droplet model is used to determine the evaporation of airborne drops contributing to in the enthalpy balance of the cloud, rather than to directly determine the initial liquid rainout fraction (although if 'rainout' is specified as the droplet fate by the user, then all remaining un-evaporated aerosol is added to the pool).

46. ACE assumes a log-normal droplet size distribution together with a fit to the mean drop diameter as a function of superheat temperature obtained from CCPS experimental data on *chlorine*. A correction is included for the effect of padding overpressure for downward releases. The CCPS experiments were for continuous releases through nozzles. Applying the ACE correlation to catastrophic failure involving substances with properties (latent heat, specific heat, surface tension) differing from those of chlorine is questionable.

47. Since the development of ACE there have been new experimental data and correlations for published for droplet sizes (see [14], [15], [16] and [17]). Much of this newer work is for aerodynamic break-up of liquid releases through orifices. However, some of this newer work covers also flashing break-up of superheated liquid releases which may be relevant also to catastrophic failure.

48. In the original ACE model it was assumed that the entire liquid inventory evaporated within the cloud. In the revised version [5] evaporation of droplets is modelled using equations for heat and mass transfer for a range of drop sizes. However, ACE does not model the variation of the droplet temperature with time, instead assuming that the drops maintain the initial superheat temperature. Whether this is a good or a poor approximation will depend on the size of the droplets and how long they are airborne – for large droplets that are airborne for a short time the assumption may be reasonable, for small droplets which remain airborne longer then this assumption may be poor.

49. Liquid rainout in ACE is modelled independently of the liquid droplet sizes, based simply on the calculated airborne fraction (see Section 4.3.2 above) and a user input option which specifies whether all the aerosol is rained out or none (see Section 4.3.6 below).

50. In our view the ACE liquid droplet model is overly complicated in some parts, overly simplistic in others and overly reliant on CCPS chlorine release data from nozzles, making its application to catastrophic failure and other substances uncertain. Fortunately, the liquid droplet model in ACE is expected to have limited impact on results, possibly altering slightly the temperature and liquid content of the cloud at the transition point to the dispersion model.

4.3.4 Enthalpy and Phase Balance

51. As discussed above, the enthalpy and phase balance equations include a coupling to the droplet model. There is also a coupling to the liquid pool, dependent upon the user selected pool option. This coupling to the liquid pool is simplified in that it assumes either

- The pool does not vaporise at all, or
- The pool completely vaporises at the boiling temperature (where the heat to maintain this boiling temperature is assumed to come from the ground).

52. The above approximations are regarded as reasonable alternative simplifications for the effect on the cloud of evolution from a pool over the short duration (typically less than 10 s) of the initial cloud expansion. A greater concern is the neglect/inclusion of the vaporisation from a pool over the longer duration associated within the subsequent dispersion modelling (see Section 4.4 for further discussion).

4.3.5 Cloud Momentum

53. As the expanding cloud mixes with ambient air it will gain momentum due to the air moving at the wind speed. ACE assumes that the average cloud velocity $\overline{v_c}$ is given by:

$$\overline{v_c} = 0.6\,(1 - c)\overline{v_w} \qquad (4\text{-}11)$$

where

c is the volumetric concentration in the cloud;

$\overline{v_w}$ is a weighted average of the wind speed over the height of the cloud.

54. The above form seems reasonable, although the weighting to give the form for $\overline{v_w}$ in [5] is not obvious. No atmospheric stability wind speed corrections are included in equation for $\overline{v_w}$. [5] refers to the 0.6 as an entrainment efficiency – this seems to be similar to empirical factors sometimes included in the advection speed of dense gases.

55. ACE calculates the displacement of the centre of cloud by approximating the motion as a constant acceleration from rest (distance = $\frac{1}{2}\overline{v_c}t$).

56. Despite some uncertainties in the precise derivation of $\overline{v_w}$, because of the short time duration, the effect of these on the displacement of the cloud is expected to be small.

4.3.6 Pool and Aerosol Options

57. ACE may be run with the following pool and aerosol options:

1. Pool formation: whether to allow pool formation
2. Fate of droplets:
    a. Aerosol: entire airborne fraction as evaporating droplets
    b. Rainout: all liquid droplets assumed to rainout as a pool
    c. Vaporisation: all droplets assumed to be completely vaporised
3. Fate of liquid pool:
    a. Pool completely vaporised at end of turbulent growth phase , or
    b. Pool vaporisation completely neglected.

58. Figure 4-4 illustrates the possible pool and liquid droplet fates in ACE.

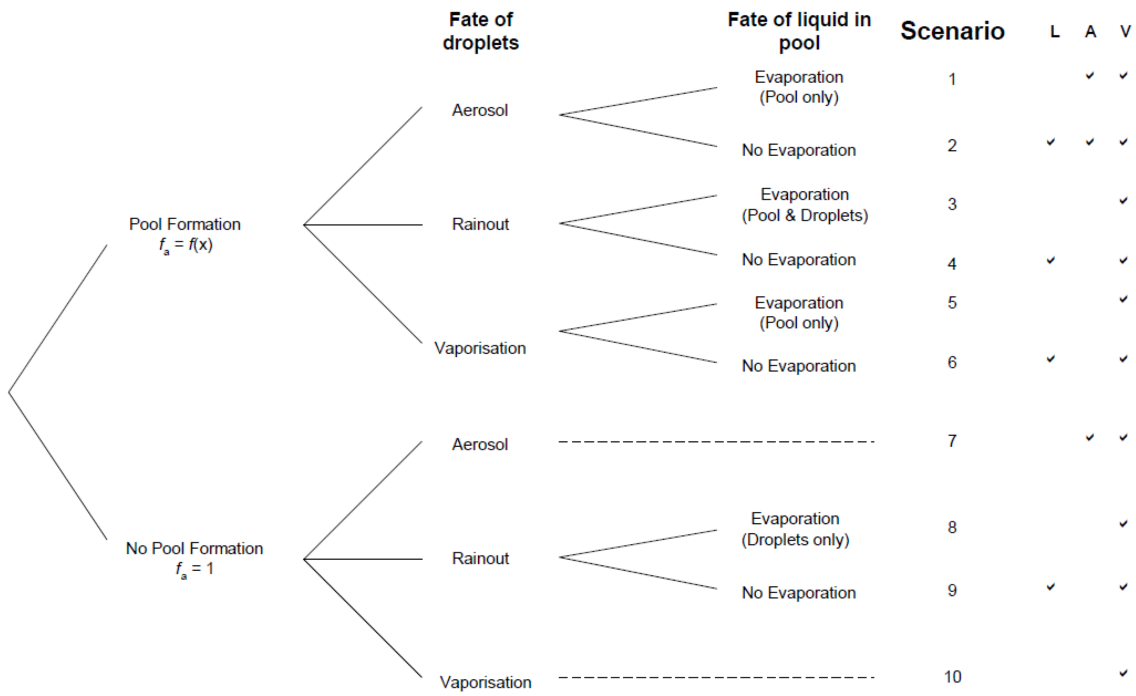

Figure 4-4 Pool and Droplet Fates in ACE from [5]. Phases present in final ACE output: L: liquid pool; A: aerosol; V: vapour.

59. Pool formation refers to the *initial* pool formation on release. If pool formation is set to 'no' there is no initial pool formation: all the liquid after flashing is assumed to be present initially as droplets. If set to 'yes' then an initial pool is formed based upon the calculated airborne fraction.

60. Droplet fate determines the subsequent fate of the droplets. 'Aerosol' assumes that any drops remaining at the end of the turbulent phase remain airborne as liquid aerosol. 'Rainout' causes any remaining drops at the end of the turbulent growth phase to be added to the liquid pool. 'Vaporise' causes an extra amount of air to be added to vaporise any remaining droplets at the end of the turbulent growth phase.

61. Pool evaporation determines whether any liquid in the pool at the end of the turbulent growth phase is to be evaporated into the cloud with the heat drawn from the substrate or whether it remains as liquid in the pool.

62. We note that ACE does not calculate pool vaporisation: the pool is either assumed to not vaporise at all over the duration of the ACE simulation, or to completely vaporise. In our opinion these are reasonable simplifications given the short duration of expansion phase and the difficulty of coupling ACE to a vaporising pool model.

63. The above combination of pool and aerosol options gives ACE flexibility in dealing with different scenarios and interfacing with different dispersion models. This flexibility is at the expense of the user having to select the most appropriate combination, not all of

which have a good physical basis. We discuss this further in Section 4.4 where we consider the most appropriate ACE options for use with DRIFT Version 3.

4.3.7 Release Directionality

64. ACE offers the choice of modelling the release as either

- Downward, or
- Omni-directional

65. Selection of the downward option results in a hemispherical cloud geometry (due to the assumption that any vapour in the (ullage) space above the liquid pushes material downwards). In this case ACE selects a lower airborne fraction (the lower curve in Figure 4-3). These options affect the airborne fraction assumed by the model. The comments here refer to the [5] version of ACE; the coupling of these options has subsequently been changed as described in Section 6 of this review.

4.3.8 End of the Turbulent Growth Phase

66. ACE terminates when the cloud turbulence characteristic velocity becomes comparable with the gravitational slumping velocity scale. At this point it is reasonable that the subsequent behaviour is modelled using a standard dense gas dispersion model including gravity slumping.

67. The transition criterion used in ACE is

$$k = \frac{3gM_v}{2\rho_a V^{2/3}} \tag{4-12}$$

where

g is the acceleration due to gravity (ms^{-2})

M_v is the mass of material (airborne) in the cloud (kg)

V is the cloud volume (m^3)

68. The transition criterion equation (4-12) is an approximation relying on the cloud being sufficiently dilute that its molar volume is similar to that of the surrounding air. This approximation may not hold, especially for large releases including aerosol. However, the effect of this is probably not too significant compared with the uncertainty in *k*.

69. The effect of equation (4-12) is that larger releases terminate sooner (at higher *k*) giving less initial dilution. This is physically reasonable and is why the assumption made by some simple models of a dilution equal to a fixed multiple of the flash fraction does not hold for the ACE predictions. The effect of equation (4-12) is evident in the results comparisons shown in Appendix A of this report.

4.3.9 Validation of the Turbulent Growth Sub-Model

70. [4] states that "…validation of the turbulence sub-model would probably be difficult to obtain, since the initial (turbulent velocity and length scale) could not be properly characterised. It is considered that the fitting to CFD calculations, as described above, would be the best that could be achieved. As with the explosion phase, it would be appropriate for the model to remain under review and to be adjusted if necessary as further relevant information, either experimental or computational, became available."

71. Comparisons with CFD predictions are given in [4]. Given the complex nature of the flashing instantaneous releases, modelling these using CFD, especially given the CFD simulations were undertaken well over 10 years ago, is extremely challenging. In our opinion, in the absence of other supporting evidence, e.g. validation against experiment, then the CFD results should be viewed as having an uncertain basis and cannot necessarily be relied on to set ACE model parameters.

72. Having said that, the trends reported CFD modelling seem qualitatively reasonable in that:

- For the glass sphere tests there is rapid expansion followed by slower growth;
- The volume at the end of the rapid expansion phase approximately scales linearly with mass;
- The turbulence velocity is dependent on the release mechanism – being higher for a release jetting through an opening/unfolding tanking as compared with an instantaneous release from a shattered glass vessel.

73. The revised ACE model, taking a user input turbulence velocity scale with a default of 10 m/s provides a more cautious approach that is welcome given the identified uncertainties in the model and limited available experimental data.

74. However, the lack of experimental validation and the reliance on uncertain CFD predictions for setting model parameters is a concern. Just because the model uses turbulent scales that are not readily obtainable from experiment does not necessarily mean that useful comparisons of bulk model predictions with data (e.g. for the time dependent growth of radius) cannot be made. We therefore suggest that there is merit in seeking to identify if there is any published experimental data, or models fitted to such data, against which the turbulent growth predictions of ACE could usefully be compared. There may also be benefit in comparing predictions from ACE with other, possibly simpler to interpret, expanding cloud models. Subsequent, and as a consequence of this review, further validation of ACE has been undertaken by HSL as reported in [2].

4.4 Recommended ACE Options for Use with DRIFT Version 3

75. In this section we consider the most appropriate ACE run options for use when DRIFT Version 3 is to be run as the subsequent dispersion model. The recommendations presented here refer to the [5] version of ACE.

76. ACE can write its results to a DRIFT Version 2 input (.DIN) file, which may then be read as a legacy file in DRIFT Version 3. Alternatively, ascii file output from ACE could be read using Excel VBA and the input data passed through to DRIFT Version 3 via its COM interface.

77. Use of the DRIFT Version 2 (.DIN) file format limits substances to either ones present in the SRD/ESR Substance database or to have their properties specified in the .DIN file as a DRIFT user defined substance.

78. The DRIFT Termination Criteria written by ACE are optional for DRIFT Version 3, which terminates its run based on the selected target dose or concentration criteria.

79. The selection of omni-directional or downward releases: In ACE this determines the airborne fraction for aerosol and the geometric factor for the cloud volume based on either spherical or hemispherical expansion in air. As already mentioned in Section 4.3.2, the association of the two curves in Figure 4-3 with omni-directional and downward releases is open to question and these two curves might more reasonably be regarded as a measure of the spread of the experimental data. If one of these two curves is to be selected as a basis for aerosol content, then we would prefer to select the upper curve – the upper curve is closer to the “rule of thumb” of three times the flash fraction and is in accord with observations that superheated releases with flash fractions of 0.3 or higher generally result in negligible pool formation. The omni-directional option also implicitly selects the geometric factor appropriate for a spherical cloud. Arguably, a hemispherical cloud is the more appropriate geometry for a large expanding release near the ground. It is not possible (without a change to the coding of ACE) to use both the upper aerosol fraction curve and the hemispherical geometry factor. The difference between the hemispherical and spherical geometry factors is at most a factor of two in the cloud volume – a difference that will soon be lost as the cloud subsequently dilutes. However, the effect of aerosol fraction can persist longer (due to it affecting material deposited from the cloud and also the evaporative cooling in the cloud). For the above reasons we recommend that the omni-directional ACE option should be used as the default in DRIFT. Consideration might also be given to altering ACE such that the upper aerosol fraction curve could be used together with a hemispherical cloud (the disadvantage being that the revised model will then differ from that published in [5]).

80. DRIFT will approximate the output from ACE as being an instantaneously released cloud. The initial displacement of the cloud as calculated by ACE (Version 2.1.0) is not transferred to DRIFT. Due to the short expansion duration, this initial displacement is likely to be a small distance which can safely be ignored in most circumstances. DRIFT will calculate the initial cloud speed based on the amount of air present in the cloud.

81. Since DRIFT is capable of modelling aerosol clouds, and airborne droplets are expected to be present (at least initially) from flashing releases, it seems most appropriate to select ‘Aerosol’ as the droplet fate. This will pass any remaining aerosol into the DRIFT initial cloud rather assuming that it all forms a pool, or arbitrarily mixing in extra air at the source to completely vaporise it. DRIFT will calculate the vaporisation of the aerosol as the cloud further mixes with air.

82. The selection of the pool formation and pool evaporation options is less clear. Possible approaches are suggested below:

1. Setting pool formation to 'no'. [5] argues that setting the pool formation to 'no' is worst case since it maximises the pollution concentration in the cloud. However, this is not necessarily the same as maximising toxic dose which depends also on the exposure duration which is influenced also by cloud passage time. Setting pool formation to 'no' together with droplet fate as 'Aerosol' will force all the liquid to be present initially as aerosol. The main objection to this is that it unrealistically excludes the formation of pools which is expected to be significant at low flash fractions – consequently it is not in accord with observations in Figure 3. Using this setting may lead to the initial DRIFT cloud being overly dense since it has too much aerosol.

2. Setting the pool formation to 'yes'. This is attractive since it reflects the realistic possibility that a pool may form (particularly important at low flash fraction). One then has to decide whether the liquid pool at the end of the ACE run is to remain as a pool or whether it is to be vaporised by ACE (taking its heat from the substrate). It is tempting to think that specifying the pool to be completely vaporised is worst case. However, as mentioned above for toxic dose, the effect of toxic exposure duration makes this open to question. If it could be shown, e.g. by running GASP (a vaporising pool model used by HSE), that the pool vaporised, or mostly vaporised, in a time less than the arrival time of the instantaneous cloud then it seems reasonable to set the ACE pool evaporation option to 'yes'. If the pool vaporised over a much longer time, then the cloud from the vaporising pool could be considered as producing a separate cloud that might give, depending on toxicity and volatility, a greater or smaller hazard range than from the instantaneous cloud. In this latter case a possible approach is to use the worst case DRIFT run from the pool vaporisation and instantaneous release – this has the merit of representing the consequence from the most appropriate source when one dominates over the other, but may not represent combined results so well where the hazard ranges from each are similar.

3. Undertaking multiple GASP and DRIFT runs as suggested above might be considered too awkward. If the number of catastrophically released pressure liquefied gases of interest is limited, then it might be possible to undertake sensitivity runs with the aim of establishing a rule set to be followed in each case, e.g. to establish conditions under which it is clear that the influence of the pool can be ignored and hence removing the need for undertaking GASP and the associated DRIFT dispersion runs in these circumstances

4. A possible future enhancement of the DRIFT model which would simplify the above process and provide a better scientific modelling basis would be to enable DRIFT to simultaneously model the dispersion from a direct source (e.g. instantaneous or continuous release) together with the dispersion from a vaporising pool. This might be done using similar cloud concentration superposition simplifications as employed in DRIFT's time-varying dispersion model.

83. To summarise, the outcome of the above considerations is that the following ACE options are recommended for use with DRIFT 3

1. Omni-directional;

2. Aerosol;

3. Pool formation: Yes;

4. Pool vaporisation: No (GASP run, or sensitivity runs are preferred to estimate the importance of vaporisation);

5. Turbulence velocity scale: ACE default of 10 m/s : the value of this is uncertain, however the validation work in [2] finds that the experimental data provide insufficient basis to replace this by an alternative value.

84. Suggested sensitivity runs illustrating the effect of selecting different ACE options for DRIFT (avoiding clearly unphysical options) are:

 1. Omni versus downward (assuming pool formation);

 2. Pool vaporisation on versus pool vaporisation off;

 3. DRIFT results from GASP simulations of the vaporising pool compared with DRIFT results from the instantaneously released airborne fraction.

5 Conclusions

85. The ACE model as presented in [4] modified in [5] has been reviewed. In conclusion, for this version of the model:

1. The model comprises of a rapid expansion phase based upon a previously published model [6] followed by a turbulent growth model newly developed for ACE.

2. The Shield model was originally developed for predicting BLEVE fireballs and is largely based on observations from videos of large scale LPG tests. This model has the merit of giving radii which are claimed to be in approximate accord with experiments covering a range of scales and fluids (mainly LPGs).

3. As pointed out in [4] the nature of the vessel failure could change the turbulence length scale, but this cannot reliably be quantified. The change to the default turbulence velocity scale in the revised version of ACE [5] does not significantly affect the final radius in the rapid growth phase (although the timescale will be lengthened), but has the effect of reducing the dilution, i.e. being more cautious, in the subsequent turbulent growth phase.

4. The turbulent growth phase of the model is tuned to uncertain CFD predictions and no experimental validation of the model is presented in [4] or [5]. The use of the 10 m/s default turbulence velocity scale in the revised ACE is considered more cautious (resulting in initially more compact clouds with less dilution) than adopting the calculated value (typically ~35 m/s) from the Shield model. In the absence of further validation then the more cautious value of 10 m/s is preferred. This has been considered in further ACE validation studies undertaken by HSL [2].

5. The droplet size modelling in ACE is tuned to chlorine release data and may not be applicable to substances with different liquid heat capacities and latent heats of vaporisation. The droplet size and evaporation modelling is in our view disproportionately detailed given the other simplifications in the modelling (e.g. the modelling of airborne fraction and the assumption of a fixed droplet temperature). This may lead to added uncertainty in the final cloud temperature and liquid content, but this is regarded as having lesser importance than the other modelling uncertainties.

6. The ACE model terminates when the turbulence velocity scale is predicted to have decayed to be comparable with the gravity slumping velocity scale, at which point output is written to DRIFT. This is an appropriate, albeit approximate, termination condition.

7. Recommendations for ACE model options to use with DRIFT Version 3 are given in Section 4.4 of this report. These may benefit from additional sensitivity analysis, guidance on the selection of which is also given in Section 4.4.

8. The limited experimental validation of ACE presented in [4] and [5] together with reliance on uncertain CFD predictions for setting model parameters in the turbulent growth model in ACE is a concern. We recognise that this is largely due to the limited experimental data available for such releases. New validation work undertaken by HSL [2] in parallel with this review compares ACE predictions with existing published experimental data covering a wide range of scales.

9. Given the identified uncertainties in the modelling, then there is potential for an integral model/correlation to be developed which is much simpler than ACE and which covers both the rapid and slower expansion phases in a unified way. The advantages of this would be:

    a. Simplicity of implementation;

    b. Clear closure assumptions;

    c. Easier validation against time dependent data;

    d. Similar, or improved, agreement with experimental data as compared with ACE.

10. However, as in ACE, the predictions of such a model can only be validated by comparison with limited available experimental data.

6 Addendum

86. In response to the findings of this review a modified version of ACE (Version 3.16) has been developed by HSL. The new version of ACE includes the following changes:

    - The omni- and down- directional options are decoupled from the upper and lower airborne fraction curves, therefore allowing the default options to be a hemi-spherical (down) cloud with the upper airborne fraction as recommended in this review.

    - The implementation of the termination criterion has been changed based upon the considerations in Appendix B of this report.

    - ACE now outputs DRIFT Version 3 (.drift) files for more robust transfer of data to DRIFT.

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Appendix A Comparisons of Predictions of ACE, IRATE and a Simple Measure

87. Calculations have been performed to compare the predicted mass of air entrained in ACE and IRATE version 3 (an instantaneous source term model used previously by HSE) for chlorine and ammonia for range of release masses. The results are shown in Figure A- 1 and Figure A- 2 including the power law fit parameters for the ACE and IRATE results.

88. The ACE runs are using defaults of an omni-directional release, 10 m/s turbulence velocity scale, pool formation and droplet aerosol formation.

89. Also shown in the figures is the line corresponding to 80 times the flash fraction. 80 times the flash fraction has no particular significance, other than it agrees fairly closely with the 10^6 kg ACE result and shows the effect of a linear relation between mass of entrained air and flash fraction.

90. Both ACE and IRATE show a power law dependence on release mass which is less than linear (power less than 1). Deviation from linear behaviour is expected in ACE due to the earlier onset of the gravity slumping termination criteria for larger releases. Without more detailed investigation it is unclear whether the turbulent growth phase model in ACE also contributes to this less than linear behaviour.

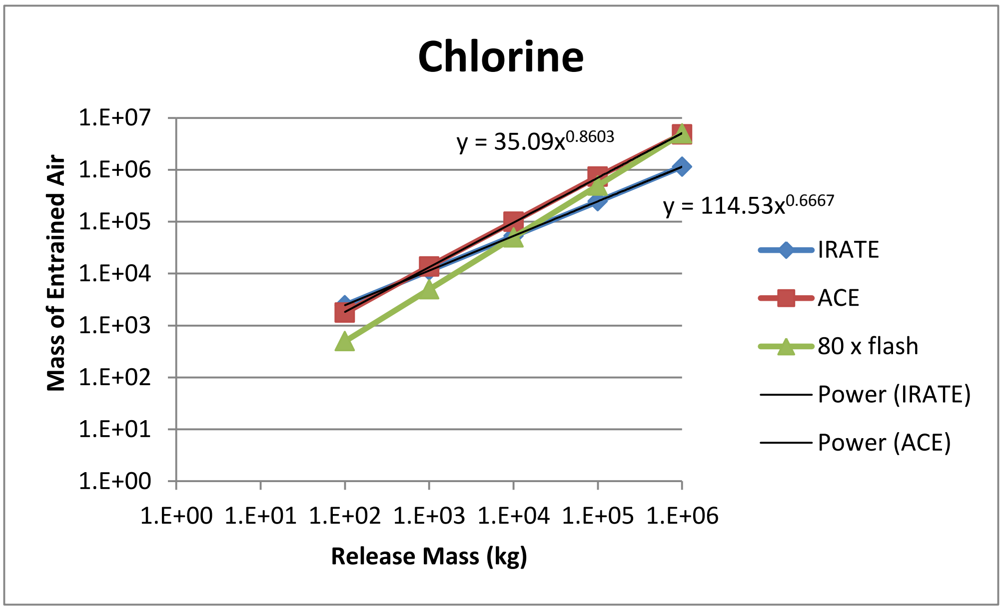

Figure A- 1 Mass of Entrained Air as a Function of Release Mass for Chlorine

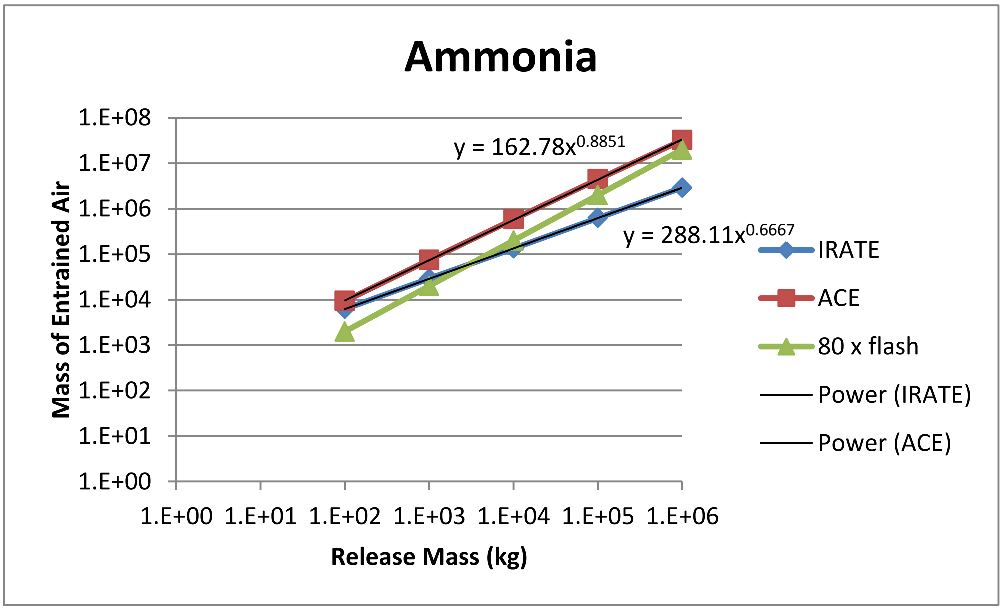

Figure A- 2 Mass of Entrained Air as a Function of Release Mass for Ammonia

Appendix B Checks on the Termination Criteria in ACE

B.1 Introduction

91. ACE Versions 3.04 and 3.1 for instantaneous release of pressure liquefied ammonia indicate significantly more air entrainment at the point of termination of ACE and transition to DRIFT. GT Science & Software was asked to investigate this further to attempt to understand why and whether there is a good basis for this behaviour. This appendix documents the findings of this investigation.

B.2 Analysis

92. The transition criterion in the ACE reports [4], [5] is where the turbulent kinetic energy, *k*, is predicted to fall below a characteristic scale for gravity slumping given by

$$k_f = \frac{3gM_v}{2\rho_a V^{2/3}} \qquad \text{(B-1)}$$

where

g is the acceleration due to gravity (m s^{-2})

M_v is the mass of contaminant material (airborne) in the cloud (kg)

V is the cloud volume (m^3)

ρ_a is the ambient air density (kg m^{-3})

93. As noted earlier in this review this criterion "…is an approximation relying on the cloud being sufficiently dilute that its molar volume is similar to that of the surrounding air. This approximation may not hold, especially for large releases including aerosol. However, the effect of this is probably not too significant compared with the uncertainty in *k*."

94. Checking the ACE source code, we note that as implemented in version 3.1, rather than (B-1) being calculated from the cloud conditions at each time step during the turbulent expansion phase this equation is evaluated prior to the turbulent expansion time step loop. Furthermore, within this equation, the software implementation uses variables from the explosion sub-model corresponding to

M_v equal initial flash fraction times the mass of the release

V equal to the cloud volume at the end of the explosive expansion phase

95. The above explains the observed behaviour for ACE predictions of ammonia – the cloud volume at the end of the explosive expansion phase is directly proportional to saturated volume of initially flashed vapour (at the boiling temperature and ambient pressure). For a similar initial flash mass fraction and similar boiling temperature then the saturated volume depends mainly on the reciprocal of the substance molecular weight. The low molecular weight of ammonia (17), for example compared with chlorine (71) gives rise to a much larger value of *V* and

consequently a smaller k_f and later termination of ACE spreading and mixing with a greater quantity of air.

96. The interpretation of M_v and V as implemented in the ACE version 3.1 source code does not seem to be correct. It would be more appropriate to base these on the airborne mass and changing cloud volume during the turbulent growth phase[1]. Furthermore, there is also the concern indicated in main review that an assumption used in the derivation of equation (B-1) may not hold for large releases including aerosol. To consider this further it is instructive to go back to derivation of equation (B-1) given in Section 6.1 of Appendix 6 of [4].

97. A characteristic scale for the gravitational slumping velocity of the cloud is

$$v_f = \left[\frac{\Delta\rho}{\rho_a} gh\right]^{1/2} \quad \text{(B-2)}$$

where

h is the characteristic height of the cloud, which is approximated by $V^{1/3}$ (m)

$\Delta\rho$ $= \rho_c - \rho_a$ where ρ_c is the characteristic cloud density (kg m^{-3})

98. By analogy with turbulent kinetic energy [4] defines

$$k_f = \frac{3}{2} v_f^2 = \frac{3}{2}\frac{\Delta\rho}{\rho_a} gh \quad \text{(B-3)}$$

and uses the approximation

$$\frac{\Delta\rho}{\rho_a} \approx \frac{M_v}{V\rho_a} \quad \text{(B-4)}$$

99. Approximation (B-4) only makes sense if M_v is the airborne mass of contaminant material (vapour plus droplets) in the cloud and V is the cloud volume which grows with time.

100. To better understand approximation (B-4) we explicitly considering the mass air M_a in the cloud which contributes to the density via

$$\rho_c = \frac{M_v + M_a}{V} \quad \text{(B-5)}$$

101. The relative density difference is therefore

$$\frac{\Delta\rho}{\rho_a} = \frac{M_v + M_a}{\rho_a V} - 1 \quad \text{(B-6)}$$

[1] It is possible that the source code implementation is a hangover from an assumption of buoyancy conservation which is an approximation for isothermal mixtures of gases, or thermal mixtures of gases with similar specific heats.

and approximation (B-4) results only if

$$M_a \approx \rho_a V \qquad \text{(B-7)}$$

102. The mass of air in the cloud is calculated in ACE by solution of quadratic equations derived from the partial pressures of material in the gaseous state and an enthalpy balance. We expect approximation (B-7) to hold when the cloud and the ambient air have similar molar volumes, which in general requires very dilute clouds (having similar temperature to air) with little or no aerosol.

103. It is not clear why the approximation (B-4) needs to be made at all, since during the turbulent expansion phase of the model there should be sufficient information to compute ρ_c directly from equation (B-5) as long as the contribution to mass of the droplets is included. Then instead of (B-4), one could simply use

$$\frac{\Delta\rho}{\rho_a} = \frac{\rho_c - \rho_a}{\rho_a} \qquad \text{(B-8)}$$

in (B-3) which is less restrictive.

B.3 Summary

104. The observed behaviour of ACE mixing in more air for ammonia than for other, higher molecular weight, substances is understood in terms of the current source code implementation of the termination criterion in ACE.

105. The source code implementation of the termination criterion in ACE 3.04 and 3.1 is based on the initial flash mass and conditions at the end of the explosive expansion phase. It is suspected that this is based on a misinterpretation of the model variables. It may be more appropriate to consider the full airborne mass of the cloud and the growing cloud volume to be used as the basis for the calculation of excess density in the termination criterion. This would necessitate the termination criterion being re-evaluated within the turbulent growth time step loop of the code.

106. Furthermore, writing the termination criterion in terms of a directly calculated relative density difference may be preferred to the dilute cloud approximation currently used within ACE.

107. The above represent straightforward modifications to ACE source code. These modifications have the potential to change, possibly significantly, the termination point and hence the dilution with air calculated by ACE.