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Review and Comments on the Models IRATE and CREATE

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QA Sheet

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1 Acronyms and Definitions

Acronym	Definition
CREATE	Continuous release source model used by HSE
DRIFT	Dispersion model developed for HSE by ESR Technology
EJECT	Jet source term model developed for HSE by AEA Technology
HSE	Health and Safety Executive
HSL	Health and Safety Laboratory
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. CREATE and IRATE are source term models used by HSE for modelling flashing continuous and instantaneous releases to provide input conditions for subsequent dispersion analysis. HSL has undertaken an initial review of these models on behalf of HSE. Although the equations of the models are documented, the physical basis of the model equations is less clear. As part of the work package aimed at characterising source terms suitable for DRIFT Version 3, Graham Tickle of GT Science and Software has been asked to undertake a quick review and to provide his comments on the model equations, with a particular emphasis on understanding the modelling basis. The aim is to provide input information to assist HSE in judging the appropriateness of these models for continued use. This report is a record of the findings of this initial review.

3 CREATE

2. The main equations for CREATE as implemented in the Visual Basic code (CREATE3v1_2) have been documented [1] and it is the gas dispersion aspects of equations that are reviewed here – the substance property correlations have not been checked as part of this initial review. Some of the same equations are also found in [2].
3. Para 35 of [2] indicates that the two-phase jet equations in paras 35 and 36 are intended to calculate the conditions of the jet at the transition point where all the liquid droplets have vaporised. [2] also gives equations for vapour jet dispersion. The equations in [2] are almost identical to those in CREATE. CREATE may be run for either two-phase releases, or choked vapour releases. The termination condition for CREATE corresponds to one of the following:
 - all the contaminant liquid has vaporised at a point where the jet velocity is below the wind speed
 - all the contaminant liquid has vaporised and the resulting vapour jet has slowed to the wind speed
 - the choked vapour jet has slowed to the wind speed.
4. Figure 3-1 shows schematically the different regions of the modelled jet:
 - The flashing region is where rapid flash vaporisation and depressurisation of the superheated liquid occurs. The end of the flashing region corresponds with reaching atmospheric pressure. Mixing with air is neglected over this region and vapour liquid equilibrium at the end of this phase implies that the jet is at the normal boiling temperature at the end of this region. The conditions at the end of the flash depressurisation region form the basis (via conserved fluxes) for describing the subsequent two-phase jet dispersion where the two-phase mixture dilutes with air. The conditions at the end of the flashing region are commonly referred to as 'expanded' or 'equivalent' conditions.
 - Two-phase dispersion region and mixing with air. In this region the ambient pressure two-phase jet entrains air and the contaminant liquid further vaporises as a result of mixing with (usually) warmer atmospheric air. Over this vaporisation region the jet will cool below the normal boiling point due to the latent heat of vaporisation being extracted.
 - Vapour jet dispersion. If the two-phase jet is predicted to dry-out by vaporising all the contaminant liquid before it has slowed to below the wind speed, then there will be a vapour jet region. Alternatively a sonic vapour release can be specified - in which case there is an expansion zone corresponding to the jet depressurising to atmospheric pressure followed by ambient pressure vapour dispersion.
 - CREATE does not include atmospheric water and therefore the influence (heating and cooling) due to water condensation and evaporation are neglected. Overall, the

neglect of water is not a concern, unless one is modelling substances which interact with water, or are borderline buoyant.

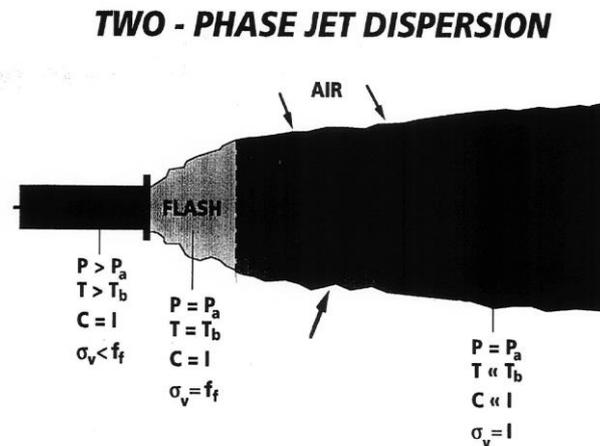


Figure 3-1 Two-phase jet model regions - from [2]

- The above approach of considering the expanded flash region followed by an entraining jet region is accepted for simplified two-phase modelling e.g. [3]. However, the simple jet dilution correlation neglects gravity and crosswind effects - these can be significant for two-phase releases. These are included in more sophisticated jet models (e.g. PHAST, EJECT).
- Below we comment on the main equations as given in [1]. Unless stated otherwise SI units are assumed.

3.1 Two-phase jet

3.1.1 Flash fraction

- The flash fraction equation is

$$f = 1 - \exp\left(\frac{-c_L(T_0 - T_b)}{\lambda}\right) \quad (3-1)$$

where

f is the fraction of vapour at the end of the flash region;

c_L is the liquid specific heat capacity evaluated at the midpoint between the release (stagnation) temperature T_0 and the normal boiling temperature T_b ;

λ is the latent heat of vaporisation evaluated also at the midpoint temperature.

- The above form is based on an isentropic flash – this is a generally accepted approximation. Alternative assumptions could also be made e.g. [3], but they often result in similar flash fractions.

3.1.2 Expanded density

9. The expanded jet density equation is

$$\rho_{eq} = \frac{1}{\left(\frac{0.082T_b \cdot f}{MW} + \frac{1-f}{\rho_L(T_b)} \right)} \quad (3-2)$$

where

ρ_{eq} is the liquid density evaluated at the normal boiling temperature;

MW is the molecular weight of the contaminant in g/mol.

10. This is the equation for the density of a homogeneous mixture of gas and liquid at the end of the flashing zone based on the vapour behaving as an ideal gas and is in accord with other similarly based models.

11. [We note that $0.082 = \frac{1000R_m}{P_a}$ where R_m is the Universal Molar Gas Constant ($R_m = 8.31 \text{ J mol}^{-1} \text{ K}^{-1}$) and P_a is standard atmospheric pressure (101325 N m^{-2}). The 1000 factor is to convert molecular weight (g/mol) to molar mass (kg/mol)].

3.1.3 Expanded velocity

12. The expanded velocity equation is

$$u_{eq} = \frac{m_0}{A_0\rho_0} + \frac{(P_0 - P_a)A_0}{m_0} \quad (3-3)$$

where

m_0 is the mass release rate at the hole

A_0 is the area of the hole

ρ_0 is the liquid density at the hole (saturated)

P_0 is the saturated pressure at the hole

P_a is ambient pressure.

13. The above form follows from considering a simple momentum balance across the flashing region e.g. [3] and is a generally accepted simplification.

3.1.4 Expanded radius

14. The expanded radius equation is

$$r_{eq} = 0.564 \sqrt{\frac{m_0}{\rho_{eq} u_{eq}}} \quad (3-4)$$

which follows from mass conservation and is accepted. [Note: $0.564 = \pi^{-1/2}$ as required for a circular jet cross-section]

3.1.5 Transition velocity

15. The transition velocity u_t is the function of the transition distance x_t

$$u_t = \frac{u_{eq}}{1 + \frac{0.257 x_t}{r_{eq} \sqrt{\rho_{eq}}}} \quad (3-5)$$

which has the same form and similar numerical coefficient as empirical correlations for the decay of velocity with axial distance in free jets e.g. [4]. The preferred (and more dimensionally appealing) way of writing this would make the dependence on air density ρ_a explicit:

$$\frac{u_{eq}}{u_t} = 1 + \frac{0.23 x_t}{\sqrt{\frac{\rho_{eq}}{\rho_a}} r_{eq}} \quad (3-6)$$

However the numerical values from both forms would be the same. The transition distance is determined by a separate equation that we shall return to later.

3.1.6 Transition radius

16. The jet radius at the transition distance is given as a function of the transition velocity u_t

$$r_t = \frac{0.9 \sqrt{\rho_{eq}} r_{eq} u_{eq}}{u_t} \quad (3-7)$$

which follows from momentum conservation:

$$\rho_t u_t^2 r_t^2 = \rho_{eq} u_{eq}^2 r_{eq}^2 \quad (3-8)$$

but this requires that we further assume that at the transition distance the jet is sufficiently dilute that its density is approximately that of air ($\rho_t \approx 1.2 \text{ kg/m}^3$). This may not always be a good assumption, but in general should not introduce large errors.

3.1.7 Mass of entrained air

17. The mass flux of entrained air at the transition point is calculated by

$$m_a = 0.009 r_t^2 u_t T_b - \frac{29m_0}{MW} \quad (3-9)$$

For dimensional consistency the 0.009 coefficient must have units of density divided by temperature.

18. To investigate the basis of (3-9), we note that $\pi r_t^2 u_t$ is the volume flux of the jet at the transition distance (total volume of the air and contaminant passing through the jet cross-section at that distance). We would expect that the total mass flux m_t (air plus contaminant) in the jet should be equal to the mixture volume flux times the density ρ_t of the jet at that point, i.e.

$$m_t = \rho_t \pi r_t^2 u_t \quad (3-10)$$

and that the mass flux of entrained air is simply the total mass flux minus the mass flux of contaminant (which, neglecting deposition, is equal to the contaminant mass release rate m_0):

$$m_a = \rho_t \pi r_t^2 u_t - m_0 \quad (3-11)$$

If we assume that the transition point corresponds to where all the liquid has evaporated, as stated in [2], then the density of the jet is given by the ideal gas law:

$$\rho_t = \frac{M_{mt} P_a}{R_m T_t} \quad (3-12)$$

where

M_{mt} is the molar mass (kg/mol) of the jet mixture at the transition distance

R_m is the Universal Molar Gas Constant (= 8.31 J mol⁻¹ K⁻¹) and

P_a is standard atmospheric pressure (=101325 Nm⁻²)

T_t is the jet temperature at the transition point

which gives

$$m_a = \frac{M_{mt} P_a}{R_m T_t} \pi r_t^2 u_t - m_0 \quad (3-13)$$

19. Comparing equation (3-13) with the CREATE equation (3-9), we note the following differences:

1. The temperature in (3-9) is the boiling temperature, rather than the temperature at the dry-out transition (the two cannot be the same if air is entrained). We would

expect the temperature of the jet at the contaminant dry-out transition point to be less than the boiling temperature.

2. The temperature in (3-9) is in the numerator of the first term, whereas the ideal gas law requires that it should be in the denominator.
 3. The subtracted mass flux in (3-9) is not the contaminant release mass flux, but the mass flux of air having the same molar release rate. This type of subtraction is sometimes used as a 'virtual source' adjustment in passive models in which the mass flux is treated as being entirely air. It is not clear why this adjustment is being applied in this case. However, the subtraction should not introduce large errors at the transition distance since the mass of entrained air is usually much larger than the contaminant mass flux.
20. To further aid comparison with (3-9), we consider the limiting case that the jet has become sufficiently dilute that the molar mass of the jet mixture is approximately equal to that of air. In this limit (3-13) gives

$$m_a = \frac{M_{ma}P_a}{R_m T_t} \pi r_t^2 u_t - m_0 \quad (3-14)$$

where M_{ma} is the molar mass of air ($0.029 \text{ kg mol}^{-1}$). We note that

$\frac{M_{ma}P_a}{R_m} \pi = 1110 \text{ kg m}^{-3} \text{ K}$. Intriguingly, if we repeated the derivation of (3-14) but used the ideal gas equation the wrong way up (inverted), we would find that

$$m_a = \frac{R_m T_t}{M_{ma} P_a} \pi r_t^2 u_t - m_0 \quad (3-15)$$

and $\frac{R_m}{M_{ma} P_a} \pi = 0.009 \text{ kg m}^3 \text{ K}^{-1}$ which exactly matches the numerical value of the coefficient in (3-9), but results in a dimensionally inconsistent equation.

21. Based on the above it seems that CREATE's mass entrainment equation is erroneous, since
 1. It is derived using an incorrect application of the ideal gas law.
 2. The use of the boiling temperature at the transition point is not correct; rather the temperature at the dry-out transition should be used. However, the error introduced by this (see later) may not be too great.
22. As an example, we consider the particular case of a substance with a boiling temperature $T_b = 240 \text{ K}$ and a temperature $T_t = 200 \text{ K}$ corresponding to contaminant liquid dry out. Neglecting the small subtracted term, then we find that CREATE equation (3-9) gives a mass flux of air approximately 40% of that obtained from (3-14). For this particular case, CREATE would give a 2.5 times more concentrated cloud at the same transition point.

3.1.8 Transition distance

23. The transition distance is given by

$$x_t = \frac{0.004r_{eq}\sqrt{\rho_{eq}}(1-f)\lambda}{T_0 - T_b} \quad (3-16)$$

24. The transition distance is an important quantity in CREATE since it is the main factor governing the jet conditions (including dilution) at the transition point. Additionally, the transition distance provides an offset that might be used in subsequent dispersion modelling.

25. To better understand the derivation of the CREATE equation (3-16) for transition distance we include the ambient air density explicitly such that

$$x_t = \frac{0.0044r_{eq}\sqrt{\rho_{eq}/\rho_a}(1-f)\lambda}{T_0 - T_b} \quad (3-17)$$

26. Substituting for x_t using (3-17) in the transition velocity equation (3-6), gives

$$1 + \frac{(1-f)\lambda}{C_{pa}(T_0 - T_b)} = \frac{u_{eq}}{u_t} \quad (3-18)$$

where we have interpreted a resulting numerical factor of 1000 as being the heat capacity of air in $\text{J kg}^{-1} \text{K}^{-1}$.

27. Taking the dilute limit $u_t \ll u_{eq}$ and $1 \ll \frac{(1-f)\lambda}{C_{pa}(T_0 - T_b)}$ of (3-18) implies

$$\frac{(1-f)\lambda}{C_{pa}(T_0 - T_b)} = \frac{u_{eq}}{u_t} \quad (3-19)$$

28. In simple jet models, the rate of decay of velocity is approximately equal to the rate of decay of other quantities derived from conserved fluxes. Therefore (3-19) can also be assumed equal, at least approximately, to $1/c$ where c is the concentration (mass per unit mass) in the jet. Hence (3-19) implies that the termination distance corresponds to where

$$C_{pa}(T_0 - T_b)/c \approx (1-f)\lambda \quad (3-20)$$

29. Equation (3-20) represents an approximate balance between the latent heat required to vaporise the contaminant liquid remaining after flashing with the sensible heat associated with changing the temperature of air from the release stagnation temperature T_0 to the normal boiling temperature T_b . This would correspond to dry-out *only if*:

1. The stagnation temperature T_0 is the same as the air temperature, i.e. ambient temperature storage situation. The corresponding equation in [2] uses the air temperature T_a instead of T_0 .
2. The temperature at the transition point is reasonably well approximated by the boiling point T_b . In fact dry-out usually requires a temperature significantly below T_b due to the latent heat of vaporisation of the liquid contaminant and the requirement for vapour-liquid equilibrium. Hence from equation (3-20) the concentration corresponding to the dry-out may be underestimated, i.e. there may be slightly more dilution in CREATE than would be required to just vaporise all the liquid. As an example, we consider propane with $T_0 = 283$ K, $T_b = 231$ K with a dry-out temperature of approximately 220 K then, using (3-20), the concentration at transition predicted by CREATE would be approximately 20% less than obtained using the dry-out temperature. A 20% change is not a particular concern.

3.1.9 Examples

30. We have undertaken some simple scoping calculations to estimate the effect that the above noted errors in the CREATE equations may have on overall dilution at the transition point.
31. We gauge the numerical error in the mass entrainment equation by taking the ratio of the leading term in (3-9) to the leading term in (3-14), giving

$$\left[\frac{R_m}{M_{ma}P_a} \right]^2 T_b T_t \quad (3-21)$$

which has units of $m^6 kg^{-2}$. A value less than 1 implies less entrainment of air in the CREATE equation than in the corrected equation. The dry-out temperature T_t may be obtained from the dry-out temperature predicted by a DRIFT Version 3 run in dry air.

32. The error in the dilution implied by the CREATE transition distances is estimated from equation (3-20) by taking the ratio

$$\frac{T_0 - T_b}{T_a - T_t} \quad (3-22)$$

A value greater than 1 implies a greater concentration in CREATE than in the corrected equation.

33. An estimate of the overall resultant effect on concentration at the transition point is given by

$$\frac{T_0 - T_b}{T_a - T_t} \bigg/ \left[\frac{R_m}{M_{ma}P_a} \right]^2 T_b T_t \quad (3-23)$$

Note, strictly this ratio has dimensions of $kg^2 m^{-6}$, due to the dimensional inconsistency which we believe to be present in CREATE's equation (3-9). The results for some example fluids are given in Table 3-1. In most of the cases in Table 3-1 the overall effect is to give

similar dilution or less, i.e. for these cases the use of CREATE is cautious in that it would result in initially higher concentrations. An exception is hydrogen fluoride stored at a saturation temperature $T_0 = 300$ K for which CREATE's equations give about 4 times more dilution than the corrected form – this is due to the relatively high boiling temperature compared to the release temperature; however, for this case we might expect that, due to the low flash fraction, significant rainout of liquid would occur for a real release.

Table 3-1 Comparison of dilution from CREATE equations with dilution using corrected equations

Substance	Sat. temp.	Amb. Temp.	Boil temp.	Dry-out ¹	Ratio CREATE / Corrected		
	T_0 (K)	T_a (K)	T_b (K)	T_t (K)	mass of air eqn (3-21) $(m^3/kg)^2$	transition eqn (3-22)	Overall, eqn (3-23) $(kg/m^3)^2$
propane	270	288	231	190	0.36	0.40	1.12
propane	288	288	231	200	0.37	0.65	1.73
propane	310	288	231	204	0.38	0.94	2.46
chlorine	270	288	239	201	0.39	0.36	0.91
chlorine	288	288	239	202	0.39	0.57	1.46
chlorine	310	288	239	204	0.40	0.85	2.14
hydrogen fluoride	300	288	292.7	238	0.56	0.15	0.26
hydrogen fluoride	340	273	292.7	241	0.57	1.48	2.58
hydrogen fluoride ²	340	288	292.7	245.5	0.58	1.11	1.91
ammonia	270	288	240	203.6	0.40	0.36	0.90
ammonia	288	288	240	204.5	0.40	0.57	1.44
ammonia	310	288	240	206	0.40	0.85	2.13

Note:

1. Dry-out temperature is estimated from runs in dry air using DRIFT Version 3
2. The small flash fraction in this case would make it very likely that, excepting a high pressure release through a very small hole, this would mainly rainout as a liquid pool

3.2 Gaseous Jet

34. In the circumstance that the user specifies a choked vapour release, or the jet velocity at the dry-out transition distance x_t is greater than the wind speed, then CREATE applies gaseous jet equations. The same gaseous jet dispersion equations are used in each case, differing only in the specification of the equivalent source conditions.

3.2.1 Dry-out of two-phase jet

35. Here the vapour jet is initialised from the conditions at the dry-out point. The model reasonably assumes that these correspond to subsonic conditions. The equivalent source conditions at the start of the vapour jet are set as follows:

- The velocity u_{eq} is set equal to the jet transition velocity u_t at the dry-out point. This is appropriate.
- The radius r_{eq} is set from the transition volume flux, v_t , in the jet using the wind speed u_w

$$r_{eq} = \left(\frac{v_t}{\pi u_w} \right)^{1/2} \quad (3-24)$$

This would correspond with the jet radius only if the jet had already slowed to the wind speed. The jet radius should instead be based on the jet velocity at the transition point u_t . This means that CREATE is assuming too large a value for r_{eq} , which has the effect of lengthening the vapour jet.

- The density is set from the total mass flux ($m_a + m_0$), the above radius r and velocity u_{eq}

$$\rho_{eq} = \frac{m_a + m_0}{\pi r_{eq}^2 u_{eq}} \quad (3-25)$$

This would be appropriate, excepting for the fact that the radius r_{eq} is set too large.

36. The wind speed transition distance, x_f is determined from

$$x_f = x_t + 14.3 r_{eq} \sqrt{\rho_{eq}} \left[0.7 - \frac{1}{\ln \left(1 - \frac{u_w}{u_{eq}} \right)} \right] \quad (3-26)$$

where x_t is the transition distance at dry-out. The above is recognised as being derived from the Kleinstein form for velocity decay of a gaseous jet e.g. [5]. Again the more standard form of this equation uses $\sqrt{\rho_{eq}/\rho_a}$ instead of simply $\sqrt{\rho_{eq}}$ with the coefficient 14.3 corresponding to an air density ρ_a of 1.2 kg/m³. This wind speed distance will be affected by the error already noted in determining r_{eq} .

37. The concentration, C , at the wind speed transition is given by

$$C = 1 - \exp \left(- \frac{1}{0.1175 \frac{x_f}{\rho_{eq}^{0.6} r_{eq}} - 0.7} \right) \quad (3-27)$$

which is approximately the Kleinstein form for a *mass* (mass/mass) based concentration, except that the dependence on ρ_{eq} is written using the 0.6 power rather than using the more standard 1/2. We note that the concentration will be affected by the error in determining r_{eq} from the jet conditions at dry-out (see above). We also note that

although the above concentration is best regarded as a mass based concentration, CREATE subsequently applies it to determine volume fluxes at the transition as if it were a volumetric (vol/vol or mol/mol) based measure. The volume based concentration should be approximately ρ_a/ρ_{eq} times the mass based concentration.

3.2.2 Choked vapour jet

38. In the case that the user specifies a choked vapour release then CREATE determines the source equivalent r_{eq} , ρ_{eq} and u_{eq} from the exit conditions, denoted here by subscript e, which are calculated from the user input stagnation conditions, denoted here by subscript 0:

39. Exit temperature:

$$T_e = T_0 \left(\frac{2}{\gamma + 1} \right) \quad (3-28)$$

This is a standard isentropic equation for ideal gas, where γ is the ratio of specific heats for the gas.

40. Exit pressure:

$$P_e = \frac{m_0}{\pi d_0^2/4} \sqrt{\frac{R_m T_0}{\gamma M_m}} \quad (3-29)$$

For clarity we've slightly rewritten the coded form in CREATE by replacing 3.6713 with $\pi\sqrt{R_m}/4$ and used the molar mass M_m (kg/mol) rather than molecular weight (g/mol).

41. To check (3-29) we derive an expression relating the exit pressure to the release rate and stagnation temperature from the standard equation, see e.g. [5], for choked vapour flow through a hole in a vessel:

$$m_0 = \frac{\pi d_0^2}{4} P_0 \sqrt{\frac{\gamma M_m}{R_m T_0} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}}} \quad (3-30)$$

and the isentropic relation

$$\frac{P_e}{P_0} = \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma-1}} \quad (3-31)$$

[which follows from $PV^\gamma = \text{constant}$ together with the ideal gas law]

42. We find that

$$P_e = \frac{m_0}{\pi d_0^2/4} \sqrt{\frac{R_m T_0}{\gamma M_m} \left(\frac{2}{\gamma + 1} \right)} \quad (3-32)$$

which differs from the CREATE expression (3-29). Our expression (3-32) is consistent with the velocity at the exit being the local sonic value as expected for choked flow. This is not the case for the CREATE expression. For typical ratios of specific heats the numerical difference between (3-29) and (3-32) is less than 10%, therefore the error in CREATE equation (3-29) should not produce significantly different results.

3.2.3 Enthalpy balance

43. The final temperature of the gaseous jet is calculated using an enthalpy balance based on the entrained air and the temperature of the released gas at ambient pressure assuming isentropic expansion. This is appropriate, but we note that, for some unknown reason, this temperature is based on a ratio of specific heats equal to 1.3, rather than taking the value determined from the substance property (SPI) file.

3.3 Grounded jet

44. CREATE includes the user option of specifying that the jet is grounded. In this circumstance CREATE increases the concentration by a factor of approximately 2. This can be interpreted as being equivalent to including 'reflection terms' in a Gaussian passive dispersion model to account for material that would otherwise be below ground. This is a reasonable approach in a simple model, but we note that observations of grounded jets, e.g. [4], indicate that, at least for relatively smooth surfaces, ground jet centreline concentrations may in fact decay with distance at a similar rate to elevated jets.

4 IRATE

45. IRATE is a model of a flashing instantaneous release. The model was originally developed by David Carter. The comments here relating to IRATE3 are based on the equations given in [6] and also, where applicable, the equations in [2].

4.1.1 Flash fraction

46. The flash fraction is given by

$$f = 1 - \exp\left(\frac{-c_L(T_0 - T_b)}{\lambda}\right) \quad (4-1)$$

Symbols definition are as described above for CREATE. This is based on a simple isentropic flash as in CREATE. Alternative assumptions are possible, but not expected to produce significantly different flash fractions. This form is generally accepted.

4.1.2 Mass of entrained air

47. The mass of air entrained is given by

$$M_a = \left[\frac{M c_L}{M_m \lambda} (T_0^2 - T_b^2) \right]^{2/3} \quad (4-2)$$

where

M is the release mass (kg)

T₀ is the stagnation temperature of the release (K)

c_L is the liquid heat capacity (J/kg/K)

T_b is the normal boiling temperature of the contaminant liquid (K)

M_m is the molar mass of the contaminant (kg/mol)

48. We have assumed the above units and chosen to write (4-2) in a slightly different form than in IRATE – in IRATE it is written in terms of the molecular weight Mw (g/mol) and includes a factor of 100 outside the square brackets. Rewriting in terms of M_m conveniently removes this factor of 100. However, as already noted in [6] both forms of the equation are dimensionally unsound, requiring a dimensioned coefficient outside the square brackets in order to give M_a in kg.

49. Apart from, or perhaps because of, being dimensionally unsound, the combination of variables in equation (4-2) is unusual, not being recognisably derived from concepts such as superheat or flash fraction. Without any further supporting evidence it is difficult to see that mass entrainment equation (4-2) has a scientific basis.

4.1.3 Enthalpy balance and phase balance

50. [6] presents equations solved using an iterative procedure equivalent to applying an enthalpy balance and phase balance to determine the final temperature and phase composition of the cloud. These equations appear to make physical sense and if correctly implemented in the code they should produce a cloud temperature and liquid content consistent with enthalpy conservation (based on the amount of air mixing in) and liquid content (based on vapour liquid equilibrium alone – rainout of liquid being ignored). These equations are capable of predicting cooling of the cloud below the released substance normal boiling point and subsequent warming if sufficient air is mixed in. Condensation of atmospheric water vapour is not accounted for in the model.

4.1.4 Cloud Volume and Radius

51. [6] does not present any equations for these, but states that cloud volume is set equal to the sum of the volume of entrained air, contaminant vapour and contaminant liquid. The cloud radius is then determined assuming a cylinder with height equal to the radius – this is often assumed as an approximation for pressurised releases (that may initially expand as hemispheric clouds when released in close proximity to the ground). These assumptions seem reasonable.

5 Conclusions

5.1 CREATE

1. The basis of the CREATE equations' derivation is not given and so has had to be inferred based on the stated intent of the model and on commonly adopted approaches.
2. The derivation of the mass of air entrained appears to be erroneous – being based upon an incorrect application of the ideal gas law.
3. The dry-out transition distance and dilution at this distance assume a temperature equal to the normal boiling temperature, whereas the temperature at this point will usually be significantly below this.
4. The equations require that the release stagnation temperature is the same as the air temperature.
5. The model uses a correlation for jet dilution that applies only to jets in still air, ignoring gravitational effects that are known to influence two-phase dispersion.
6. CREATE does not appear to include a liquid rainout model – in which case the model may be very conservative for low superheats which might be reasonably expected to deposit significant amounts of material as a pool.
7. Condensation of atmospheric water in the cold cloud is ignored, but this is not regarded as a serious omission, excepting perhaps for substances that interact with water.
8. Comparisons between the CREATE equations and their 'corrected' counterparts suggests that in many cases CREATE will be cautious, i.e. predict higher concentration at the transition point. However, this is not universally the case.
9. We have noted some inconsistencies in the vapour jet equations that are used in the event of a user specifying a choked vapour release, or when the two-phase release is predicted to dry-out at a speed greater than the wind speed. Mostly these are of little consequence, the exception being the setting of the equivalent radius at dry-out from the wind speed – this could significantly overestimate the length of the vapour jet if the jet still has a high velocity at contaminant dry-out.
10. In some circumstances, the dry-out transition distance in CREATE might be large, and this may be better modelled using a gas dispersion model capable of modelling aerosol. The argument for using a gas dispersion model instead of CREATE is even stronger when the dispersion model is also capable of modelling jets in a more complete way than CREATE.

5.2 IRATE

1. As for CREATE, the basis of the IRATE equations' derivation is not given in the provided documents.
2. The basis of the equation for the mass of air entrained is particularly unclear. This equation is dimensionally unsound and is not recognisably derived from concepts such as superheat or flash fraction.
3. The basis of the rest of the model is understood – in particular, unlike CREATE, IRATE seems to perform an enthalpy balance and vapour liquid phase equilibrium calculation, such that the cloud will cool below the normal boiling temperature whilst vaporising the released liquid.
4. Unlike CREATE, IRATE does not appear to assume that all the liquid must be vaporised – the final liquid content is determined by the cloud thermodynamics based upon the amount of air mixed in.
5. IRATE does not appear to include a liquid rainout model – in which case the model may be very conservative for low superheats which might be reasonably expected to deposit significant amounts of material as a pool.
6. Without the equation for the mass of air mixed into the cloud having an obvious scientific basis, or demonstrated fitting to experimental data, it is difficult to have confidence in the predictions of IRATE.
7. Comparisons with an alternative instantaneous source model ACE given in [7] suggest that IRATE entrains less mass of air than ACE, but conversely [7] concluded that overall IRATE compared well with ACE (after a retuning of ACE). Other comparisons, ideally where there is also experimental data, may be beneficial.
8. It might also be beneficial to do a more thorough literature search with the aim of identifying the origin of the air entrainment model in IRATE.
9. Based on this initial review it is not possible to state whether, or even under what circumstance, IRATE provides a conservative source term estimate. However, a model with a dimensionally unsound basis, even if agreeing with data for one fluid/scale is unlikely to extrapolate well to different fluids/scales.

6 References

- [1] A. Lamb, "HSL Summary Note on CREATE. Included as an appendix to this report.," 2012.
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- [4] N. Rajaratnam, *Turbulent Jets*, Elsevier, 1976.
- [5] F. P. Lees, *Loss Prevention in the Process Industries: Hazard Identification, Assessment and Control*, 2nd ed., Butterworth Heinemann, 1996.
- [6] H. Cruse, "HSL Summary Note on IRATE model. Included as an appendix to this report.," 2012.
- [7] A. H. Shepherd and D. H. Deaves, "Source Term Calculation for Flashing Releases - Background to the Development of ACE," WS Atkins Report No. AM5233-R1, 2000.

Appendix A HSL Summary Note on IRATE Model

A.1 Overview of the IRATE model

52. The IRATE model was originally developed by David Carter. Some of the equations (such as those for the flash fraction and the mass of air entrained) are equivalent to the equations given in the ‘flashing instantaneous release’ section of Carter (1991), but Carter does not explain their origin.

53. The flash fraction, f , is given by the following equation:

$$f = 1 - \exp\left[\frac{-C_{p,l}(T_{\text{stag}} - T_{\text{bp}})}{\Delta H_{\text{vap}}}\right], \quad \text{Eqn. \{1\}}$$

where:

$C_{p,l}$ is the specific heat of the liquid phase pollutant;

T_{stag} is the stagnation temperature;

T_{bp} is the boiling point of the pollutant; and

ΔH_{vap} is the heat of vaporisation of the pollutant.

54. Various options for calculating the flash fraction have been reviewed by Macbeth (2009). Macbeth concludes that equation {1} should only be used in integral format. Its implementation in IRATE will underestimate the flash fraction.

55. IRATE assumes that all the liquid that does not flash enters the cloud as an aerosol (in other words, the airborne fraction is 1). The mass of air entrained, M_a , is calculated by the following equation:

$$M_a = 100 \left[\frac{M C_{p,l}}{mw \Delta H_{\text{vap}}} (T_{\text{stag}}^2 - T_{\text{bp}}^2) \right]^{2/3}, \quad \text{Eqn. \{2\}}$$

where:

M is the release mass; and

mw is the molecular weight of the pollutant.

56. It is unclear how equation {2} has been derived. It does not appear to be based on the equations that appear in standard texts such as Lees (1996) or the TNO ‘Yellow book’ (van den Bosch and Weterings (ed), 2005). The factor of 100 has probably been included to convert the molecular weight from g/mol to kg/mol, but the overall equation is dimensionally incorrect.

57. IRATE uses an iterative process to calculate the temperature of the cloud (T_{cloud}) and the fraction of the liquid remaining after the adiabatic flash that is subsequently vaporised (GA).

58. At each iteration, a new value for GA is chosen and the temperature of the cloud is calculated from an enthalpy balance:

$$\begin{aligned}
 &M_a C_{p,a} (T_{\text{cloud}} - T_a) && \text{(change of enthalpy of air)} \\
 &+ GA M_l \Delta H_{\text{vap}} && \text{(enthalpy required to evaporate droplets)} \\
 &+ (M_l C_{p,l} + M_v C_{p,v}) (T_{\text{cloud}} - T_{\text{bp}}) && \text{(enthalpy required to heat vapour and liquid entrained} \\
 &&& \text{in cloud)} \\
 &= 0, && \text{Eqn. \{3\}}
 \end{aligned}$$

where:

- $C_{p,a}$, $C_{p,l}$ and $C_{p,v}$ are the specific heats of air, the liquid pollutant and the gas pollutant, respectively;
- T_{cloud} and T_a are the temperature of the cloud and the ambient air respectively;
- M_a is the mass of air entrained;
- M_v is the mass of vapour after the adiabatic flash;
- M_l is the mass of liquid remaining after the adiabatic flash; and
- GA is the fraction of the liquid remaining after the adiabatic flash that is vaporised.

59. This rearranges to:

$$T_{\text{cloud}} = \frac{M_a C_{p,a} T_a + (M_l C_{p,l} + M_v C_{p,v}) T_{\text{bp}} - GA M_l \Delta H_{\text{vap}}}{M_l C_{p,l} + M_v C_{p,v} + M_a C_{p,a}} \quad \text{Eqn. \{4\}}$$

60. The partial pressure of the pollutant is then calculated using the following equation:

$$PP = \frac{(M_v + GAM_l)/mw}{(M_v + GAM_l)/mw + M_a/mw_a}, \quad \text{Eqn. \{5\}}$$

where mw_a is the molecular weight of air.

61. The iteration continues until the partial pressure is equal to the vapour pressure of the pollutant at the cloud temperature. The volume of air in the cloud, the volume of vapour in the cloud and the volume of liquid in the cloud are then summed to give the total volume of the cloud. The radius of the cloud is calculated assuming that the cloud is a cylinder of height equal to its radius.

A.2 The key assumptions in IRATE

62. Table A- 1 summarises the main assumptions that are made within the IRATE3 model.

Table A- 1 The key assumptions in IRATE

<i>Property or process to be modelled</i>	<i>IRATE assumption</i>
Flash fraction	The flash fraction is calculated from an enthalpy balance, using equation {1}.
Airborne fraction	The model assumes that all liquid that is not initially flashed is entrained as droplets in the cloud, giving an airborne fraction of 1.
Volume of cloud	The mass of air entrained is calculated by a simple equation, which depends on the total mass released. It is possible that this equation is based on an enthalpy balance, but it is dimensionally incorrect. The cloud temperature and the fraction of the liquid remaining after the adiabatic flash that is vaporised are calculated iteratively. This allows the final mass (and therefore final volume) of vapour and liquid in the cloud to be determined. The cloud volume is the sum of the volume of vapour in the cloud, the volume of liquid in the cloud and the volume of air in the cloud.
Evaporation of droplets entrained in cloud	Droplet evaporation continues until the partial pressure of the pollutant equals its vapour pressure at the cloud temperature. This is calculated iteratively.
Cloud temperature	The cloud temperature is calculated iteratively as part of the process for calculating droplet evaporation.
Cloud momentum	Ignored
Turbulence velocity	Not used
Pool formation	Not accounted for
Growth in cloud size	The growth in cloud size is proportional to $M^{2/3}$, where M is the total mass released. This relationship arises because of the form of equation {2}, whose derivation is uncertain.
Rainout	If the superheat (stagnation temperature – boiling point of the pollutant) is less than 15 K, a message box appears stating 'liquid rainout predicted' and IRATE3 does not produce any output. If the superheat is greater than 15 K, rainout is neglected.

Helen Cruse, HSL, 25th September 2012

A.3 References

Carter DA (1991). *Source Terms*, in Risk Analysis in the Process Industries. A Three Day Workshop, 12-14 March 1991, Grosvenor Hotel, Chester, England, IBC Technical Services Ltd.

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Appendix B HSL Summary Note on CREATE Model

63. CREATE is a program written in Visual Basic and used to model two-phase jets or choked vapour releases. Here we briefly document the main equations used within the CREATE3 spreadsheet to model two-phase jets.

B.1 Flash fraction

64. The flash fraction, f , is given by the following equation:

$$f = 1 - \exp\left[\frac{-C_{p,l}(T_{\text{stag}} - T_{\text{bp}})}{\Delta H_{\text{vap}}}\right], \quad \text{Eqn. \{6\}}$$

where:

- $C_{p,l}$ is the specific heat of the liquid phase pollutant in $\text{Jkg}^{-1}\text{K}^{-1}$;
- T_{stag} is the stagnation temperature in K;
- T_{bp} is the normal boiling point of the pollutant in K; and
- ΔH_{vap} is the heat of vaporisation of the pollutant in J/kg.

65. The values of the liquid specific heat and the heat of vaporisation that are input into equation {6} correspond to temperature $T = (T_{\text{stag}} + T_{\text{bp}})/2$, and are calculated using the functions LSH(T) and DHV(T) respectively.

66. The function LSH(T) calculates the liquid specific heat at temperature T in $\text{Jkg}^{-1}\text{K}^{-1}$:

$$\text{LSH}(T) = \left[\frac{0.1745 - 0.0838(T_{\text{ref}}/T_c)}{0.1745 - 0.0838(T/T_c)}\right]^{2.8} C_{p,l}(T_{\text{ref}}) \quad \text{Eqn. \{7\}}$$

where:

- $C_{p,l}(T_{\text{ref}})$ is the liquid specific heat at temperature T_{ref} in $\text{Jkg}^{-1}\text{K}^{-1}$; and
- T_c is the critical temperature in K.

67. The function DHV(T) calculates the latent heat of vaporisation at temperature T in J/kg, using the Watson relation, as given in Reid *et al.* (1987):

$$\text{DHV}(T) = \left(\frac{T_c - T}{T_c - T_{\text{bp}}}\right)^{0.38} \Delta H_{\text{vap}}(T_{\text{bp}}), \quad \text{Eqn. \{8\}}$$

where $\Delta H_{\text{vap}}(T_{\text{bp}})$ is the latent heat of vaporisation at the normal boiling point in J/kg.

B.2 Density of gas

68. The density of gas in kg/m^3 , $\rho_g(P, T)$, is calculated by solving the Redlich-Kwong equation of state iteratively. The Redlich-Kwong equation is given in Reid *et al.* (1987) as:

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m + b)}, \quad \text{Eqn. \{9\}}$$

where:

- P is the pressure;
- R is the Molar Gas constant;
- T is the temperature; and
- V_m is the molar volume.

69. The parameters a and b take the following form:

$$a = \frac{0.42748R^2T_c^{5/2}}{P_cT^{1/2}} \quad b = \frac{0.08664RT_c}{P_c},$$

where:

- T_c is the critical temperature; and
- P_c is the critical pressure.

70. In CREATE3, the Redlich-Kwong equation of state is expressed in terms of the compressibility, $Z = PV_m/RT$:

$$Z^3 - Z^2 + (A - B^2 - B)Z - AB = 0 \quad \text{Eqn. \{10\}}$$

71. The parameters A and B take the following form:

$$A = \frac{0.42748P_r}{T_r^{5/2}} = \frac{aP}{R^2T^2}$$

$$B = \frac{0.08664P_r}{T_r} = \frac{bP}{RT},$$

where:

- $T_r = T/T_c$ is the reduced temperature; and
- $P_r = P/P_c$ is the reduced pressure.

72. In the CREATE3 spreadsheet, the compressibility, Z , is determined by using the Newton-Raphson method to solve equation {10} iteratively. The density is then calculated using the following equation:

$$\rho_g = \frac{mwP}{ZRT}, \quad \text{Eqn. \{11\}}$$

where:

- mw is the molecular weight of the pollutant in g/mol;
- P is the pressure in Pa;
- R is the Molar Gas constant in $\text{Jkmol}^{-1}\text{K}^{-1}$; and
- T is the temperature in K.

B.3 Density of Liquid

73. The density of the liquid in kg/m^3 , $\rho_1(T)$, is calculated using the following equation:

$$\rho_1(T) = \left(\frac{T_c - T}{T_c - T_{\text{ref}}} \right)^{1/3} \rho_1(T_{\text{ref}}), \quad \text{Eqn. \{12\}}$$

where $\rho_1(T_{\text{ref}})$ is the liquid density at temperature T_{ref} in kg/m^3 . Note that the reference temperature can be different to that used in equation {7}.

B.4 Saturated vapour pressure

74. The function $\text{Pres}(T)$ uses a reduced form of the Riedel equation to calculate the saturated vapour pressure at temperature T in Pa, following the methodology described in Coulson *et al.* (2002). The correlation used is:

$$\ln P_r^\circ = A - \frac{B}{T_r} + C \ln(T_r) + DT_r^6 \quad \text{Eqn. \{13\}}$$

$$\text{Pres}(T) = P_r^\circ P_c, \quad \text{Eqn. \{14\}}$$

where:

- $T_r = T/T_c$ is the reduced temperature;
- P_r° is the reduced vapour pressure; and
- P_c is the critical pressure in Pa.

75. The coefficients A to D are derived by inserting a known vapour pressure point into equation {13}. In the CREATE3 spreadsheet the vapour pressure at the normal boiling point is used for this purpose. The coefficients take the following form:

$$A = -35c_1; \quad B = -36c_1; \quad C = 42c_1 + c_2; \quad \text{and} \quad D = -c_1,$$

where:

$$c_1 = 0.0838(3.758 - c_2)$$

$$c_2 = \frac{0.315c_5 - \ln P_{r1}^\circ}{0.0838c_5 - \ln T_{r1}}$$

$$c_5 = -35 + \frac{36}{T_{r1}} + 42 \ln(T_{r1}) - T_{r1}^6,$$

where P_{r1}° is the reduced vapour pressure at reduced temperature T_{r1} . Note that in Coulson *et al.* (2002), the second term of the equation for c_5 is written incorrectly.

B.5 Expanded density

76. The expanded density, ρ_{eq} , is calculated using the following equation:

$$\rho_{eq} = \frac{1}{\left(\frac{0.082T_{bp}f}{mw} + \frac{1-f}{\rho_1(T_{bp})} \right)}, \quad \text{Eqn. \{15\}}$$

where:

- mw is the molecular weight of the pollutant in g/mol; and
- $\rho_1(T_{bp})$ is the density of the liquid at the normal boiling point in kg/m³, which is determined using the relationship given in equation {12}.

B.6 Expanded velocity

77. The expanded velocity, u_{eq} , is calculated using the following equation:

$$u_{eq} = \frac{m_0}{A_0 \rho_1(T_{stag})} + \frac{(P_{stag} - 101325)A_0}{m_0}, \quad \text{Eqn. \{16\}}$$

where:

- m_0 is the mass release rate input by the user in kg/s;
- $P_{stag} = \text{Pres}(T_{stag})$ is the stagnation pressure in Pa;
- 101325 is the atmospheric pressure in Pa;
- $\rho_1(T_{stag})$ is the density of the liquid at the stagnation temperature in kg/m³, which is determined using the relationship given in equation {12}; and
- $A_0 = \frac{1}{4} \pi D_0^2$ is the orifice area in m², where D_0 is the orifice diameter.

B.7 Expanded Radius

78. The expanded radius, r_{eq} , is calculated using the following equation:

$$r_{eq} = 0.564 \sqrt{\frac{m_0}{\rho_{eq} u_{eq}}} \quad \text{Eqn. \{17\}}$$

B.8 Transition distance

79. The transition distance, x_t , is calculated using the following equation:

$$x_t = \frac{0.004 r_{eq} \sqrt{\rho_{eq}} (1-f) \Delta H_{vap}}{T_{stag} - T_{bp}} \quad \text{Eqn. \{18\}}$$

B.9 Transition velocity

80. The transition velocity, u_t , is calculated using the following equation:

$$u_t = \frac{u_{eq}}{1 + \frac{0.257 x_t}{r_{eq} \sqrt{\rho_{eq}}}} \quad \text{Eqn. \{19\}}$$

B.10 Transition Radius

81. The transition radius, r_t , is calculated using the following equation:

$$r_t = \frac{0.9 \sqrt{\rho_{eq}} r_{eq} u_{eq}}{u_t} \quad \text{Eqn. \{20\}}$$

B.11 Mass of air entrained

82. The mass rate at which air is entrained, m_a , is calculated using the following equation:

$$m_a = 0.009 r_t^2 u_t T_{bp} - \frac{29 m_0}{mw} \quad \text{Eqn. \{21\}}$$

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B.12 References

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