Jack Rabbit III Modelers Working Group

Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials

Version 1.2, 12 January 2022

Simon Gant[1], Graham Tickle[2], Rory Hetherington[3] and Joseph Chang[4]

[1] UK Health and Safety Executive (simon.gant@hse.gov.uk)
[2] GT Science and Software (graham.tickle@gtscience.co.uk)
[3] UK Health and Safety Executive (rory.hetherington@hse.gov.uk)
[4] RAND Corporation (jchang@rand.org)

Contents

Background

The model input conditions for the Jack Rabbit III inter-comparison exercise on Desert Tortoise and FLADIS are described in the document entitled “Initial Modeling Exercise (2021-2022)” [File: JRIII initial modeling exercise description v2.3.pdf]. The document includes a description of equivalent vapor-only source conditions for five of the six trials selected for the exercise (Desert Tortoise trials 1 and 2, and FLADIS trials 9, 16 and 24). These were all taken from the SMEDIS database (Carissimo *et al*., 2001). Equivalent source conditions were not provided for Desert Tortoise 4, since the SMEDIS database did not examine that trial. The purpose of this document is to provide details of the equivalent vapor-only source conditions for Desert Tortoise 4 for the purposes of the Jack Rabbit III modeling exercise.

Summary of Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials

The conditions that are recommended to be used by modelers participating in the Jack Rabbit III exercise for Desert Tortoise are summarized in Table 1 below. The results for Desert Tortoise trials 1 and 2 (DT1 and DT2) are identical to those given in the document previously circulated [File: JRIII initial modeling exercise description v2.3.pdf].

Table 1 Recommended equivalent vapor-only source conditions for the Desert Tortoise trials for the Jack Rabbit III modeling exercise

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Temperature (K)	Half-width[a] (m)
DT1[b]	51.0	7.5	13	205	6.40
DT2[b]	48.3	6.0	13	205	8.40
DT4[c]	49.5	8.59	14.3	205	6.99

Notes:

[a] The source size has been specified this time as a rectangular window of height = the half-width.

[b] These conditions come from the SMEDIS database, https://admlc.com/smedis-dataset/. The equivalent source terms are in files “equivsrc.txt”, distributed in zip files “batch1_24.zip”, “batch2_24.zip” and “batch3_24.zip”.

[c] These are the new values calculated here using the method described in this document.

The calculation method used to determine the source conditions for DT1 and DT2 in the SMEDIS project were described in Appendix 4 of the report by CERC (2000). However, some details of the method were not given, such as the input values used in the calculation, e.g., the atmospheric pressure, the thermodynamic properties of ammonia and the assumed jet entrainment coefficient.

HSE has coded up the method described by CERC (2000) to determine the source conditions for DT4. As a verification check, to ensure the method has been coded correctly, HSE has also produced results for DT1 and DT2 (see Table 2 below). The results from HSE’s calculations are mostly within 10% of the values given in the SMEDIS database, although the velocity in DT2 calculated by HSE (7.7 m/s) was somewhat larger than the value given by SMEDIS (6.0 m/s). These differences between the HSE and SMEDIS values are likely to be due to different choices made in the inputs to the calculations. HSE has used the atmospheric pressure recorded at the China Lake test site, the NIST Webbook as a source of thermodynamic properties and an entrainment coefficient of 0.08 (further details are given below).

Due to the uncertainty in the source conditions for DT1 and DT2, it is suggested that if modelers have sufficient time, that in addition to the baseline inputs given in Table 1 for DT1 and DT2 they also run sensitivity tests using the input conditions given in Table 2. Such sensitivity tests are not a mandatory part of the Jack Rabbit III modeling exercise, but they could provide useful results.

Table 2 Equivalent vapor-only source conditions for Desert Tortoise trials 1 and 2 calculated by HSE using the method described in this document, which could be used for model sensitivity tests

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Temperature (K)	Half-width[a] (m)
DT1	46.7	7.27	13.8	205	6.63
DT2	54.8	7.70	13.9	205	7.76

[a] The source size has been specified this time as a rectangular window of height = the half-width.

Summary of CERC (2000) Calculation Method

The CERC (2000) calculation of the equivalent vapor-only source term splits the release into three stages as shown in Figure 1:

1. The first flashing stage models the expansion of the jet as the pressure drops from the elevated pressure at the orifice to atmospheric pressure at the end of the flashing stage. Since the pressure is above the ambient in this stage, it is assumed there is no air entrainment. The temperature at the end of this flashing stage is the normal boiling point of ammonia at atmospheric pressure. Conditions at the end of Stage 1 consist of a mixture of ammonia vapor and ammonia liquid droplets (with no air present).

2. During the second stage, air is entrained into the jet and the liquid aerosol droplets evaporate. This stage extends to the point where all of the liquid ammonia has evaporated. The temperature is in equilibrium with the partial vapor pressure throughout this stage, with the temperature falling as air is entrained. The aim of the present calculation exercise is to calculate the final conditions at the end of this stage, to use as input conditions for atmospheric dispersion models.

3. The final stage comprises a cold, single-phase vapor jet dispersing in air.

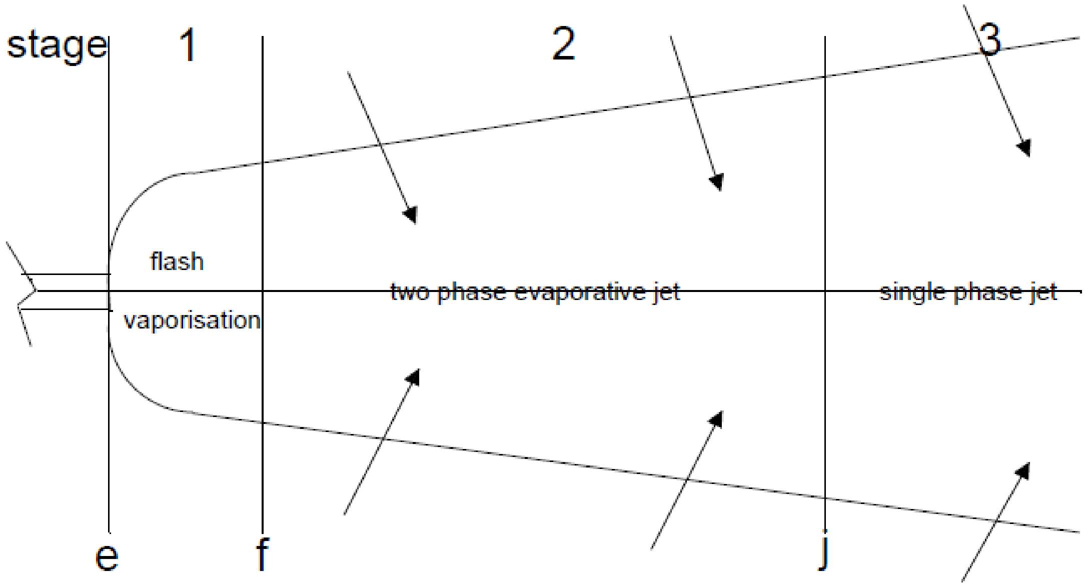

Figure 1 Schematic diagram of the two-phase jet model from CERC (2000)

A number of simplifying assumptions are used to derive the vapor-only source conditions. A top-hat distribution of concentration and velocity is assumed throughout. The air is assumed to be dry, i.e., atmospheric humidity effects are ignored. A control volume approach is used to determine conditions at the end of Stages 1 and 2, based on conservation of mass, momentum and energy (or enthalpy). Other methods of calculating conditions at the end of Stage 2 can be found in the literature (see, for example, Wheatley, 1987), but the focus here has been to adopt the same approach as that used to derive the SMEDIS source conditions, as described by CERC (2000).

Stage 1 Flash Vaporization

The conservation equations solved in the flash vaporization stage were given by CERC (2000) as follows:

Conservation of energy

$$\left[h_{vf} - \left(1 - X_f\right)H_f\right] - \left[h_{ve} - (1 - X_e)H_e\right] + \frac{1}{2}\left(v_f^2 - v_e^2\right) = 0 \qquad (1)$$

Conservation of momentum

$$\rho_e v_e\left(v_f - v_e\right) + \left(P_f - P_e\right) = 0 \qquad (2)$$

Conservation of mass

$$\rho_e v_e A_e = \rho_f v_f A_f \qquad (3)$$

In these equations, h is the specific enthalpy, X the quality (i.e., the vapor mass fraction), H is the enthalpy of vaporization, v the velocity and ρ the density. Subscript v refers to vapor and subscripts f and e to conditions at the end of the flashing stage and conditions at the pipe exit, respectively. A full list of nomenclature can be found at the end of this document.

CERC (2000) also noted that the density of the two-phase vapor-liquid mixture could be found from:

$$\frac{1}{\rho_f} = \frac{\left(1 - X_f\right)}{\rho_{lf}} + \frac{X_f}{\rho_{vf}} \qquad (4)$$

where the ammonia liquid and vapor densities at the end of flashing, ρ_{lf} and ρ_{vf}, can be found from saturation conditions at atmospheric pressure.

CERC (2000) did not identify the source of information used for thermodynamic properties of ammonia. In the present work, the NIST Webbook[1] has been used. The temperature at the end of flashing has been found here using the Antoine equation:

$$T_f = \frac{b}{a - \log_{10}(P_a)} - c \qquad (5)$$

where the coefficients $a = 3.18757$, $b = 506.713$ and $c = -80.78$ have been taken from the NIST Webbook. In the above equation, the pressure P_a is the atmospheric pressure (in bar absolute in the above NIST formula) and the temperature T is output in Kelvin. The coefficients a, b and c are valid for temperatures below the normal boiling point, i.e., from 164.0 K to 239.6 K. Values used in the present flash vaporization calculation are summarised in Table 3.

---

[1] https://webbook.nist.gov/cgi/cbook.cgi?ID=7664-41-7

Table 3 Summary of input conditions for the Desert Tortoise trials taken from file "JRIII initial modeling exercise description v2.3".pdf

		DT1	**DT2**	**DT4**	SI Units
Mass flow rate of ammonia	$\dot{m}$	80.0	117.0	108.0	kg/s
Diameter of pipe exit	D_e	0.081	0.0945	0.0945	m
Pressure at the pipe exit	P_e	1.01E6	1.12E6	1.18E6	Pa (abs)
Temperature at the pipe exit	T_e	294.65	293.25	297.25	K
Atmospheric pressure	P_a	9.09E4	9.10E4	9.03E4	Pa (abs)
Atmospheric temperature	T_a	301.95	303.55	305.55	K

The calculation then proceeds as follows. Firstly, the temperature at the end of flashing, T_f, is calculated from Equation (5) using the atmospheric pressure, P_a, given in Table 3.

The density and specific enthalpy of liquid ammonia at the pipe exit, ρ_e and h_e, are then found from the NIST Webbook using the pressure and temperature (P_e and T_e) given in Table 3. Similarly, the densities and specific enthalpies of pure ammonia liquid and vapour at the end of the flashing stage are found from the saturation properties of ammonia in the NIST Webbook at atmospheric pressure, P_a. The heat of vaporization, H_f, is found from the following correlation developed by Osborne and Van Dusen (1917):

$$H_f = 1000\left[137.91\sqrt{133 - T_f + 273.15} - 2.466(133 - T_f + 273.15)\right] \qquad (6)$$

where the temperature, T_f, in the above equation is expressed in Kelvin and H_f is calculated in J/kg. The correlation is valid for temperatures between -42 °C and +52 °C. As a verification check, values from the above correlation have been cross-checked against spot values obtained from the NIST Webbook and the two were found to match to three significant figures. The ammonia property data described above is summarized in Table 4.

Table 4 Calculated temperature at the end of flashing (from the Antonine equation) and density and specific enthalpy obtained from the NIST Webbook for ammonia

		DT1	**DT2**	**DT4**	SI Units
Temperature at the end of flashing	T_f	237.7	237.7	237.6	K
Density of liquid ammonia at pipe exit	ρ_{le}	608.3	610.5	604.5	kg/m^3
Density of ammonia liquid at end of flashing	ρ_{lf}	684.2	684.2	684.4	kg/m^3
Density of ammonia vapour at end of flashing	ρ_{vf}	0.805	0.805	0.799	kg/m^3
Specific enthalpy of ammonia liquid at pipe exit	h_{le}	4.47E+05	4.40E+05	4.59E+05	J/kg
Specific enthalpy of ammonia liquid at the end of flashing	h_{lf}	1.85E+05	1.85E+05	1.84E+05	J/kg
Heat of vaporisation of ammonia at the end of flashing	H_f	1.37E6	1.37E6	1.37E6	J/kg

The next step is to calculate the velocity at the pipe exit from:

$$v_e = \frac{\dot{m}}{\rho_{le} A_e} \tag{7}$$

where the mass flow rate, $\dot{m}$, is given in Table 3, the ammonia liquid density, ρ_{le}, is given in Table 4 and the area of the pipe exit is calculated from $A_e = \pi D_e^2/4$, using the diameter D_e given in Table 3.

This velocity at the pipe exit can then be used to determine the velocity at the end of the flashing stage, v_f, from conservation of momentum (Equation 2), which is rearranged as follows:

$$v_f = v_e + \frac{(P_e - P_f)}{\rho_e v_e} \tag{8}$$

where the pressure at the end of the flashing stage, P_f, is equal to the atmospheric pressure, P_a (given in Table 3).

The next step in the calculation process is to determine the quality (i.e., the ammonia vapour mass fraction) at the end of the flashing stage. Equation (1) expresses conservation of energy, where the first two terms in square brackets express the change in enthalpy between the pipe exit and the end of the flashing stage. The first term in square brackets can be rewritten in a slightly simpler form as follows:

$$h_{vf} - (1 - X_f) H_f = h_{lf} + X_f H_f \tag{9}$$

where, by definition, $H_f = h_{vf} - h_{lf}$. Additionally, in the Desert Tortoise trials, the fluid at the pipe exit was pressurized above the saturation vapor pressure and so the second term in square brackets in the energy equation can be simplified to just h_{le}, i.e., the enthalpy of liquid ammonia at the exit pressure and temperature (given in Table 4). The energy equation then becomes:

$$h_{lf} + X_f H_f - h_{le} + \frac{1}{2}\left(v_f^2 - v_e^2\right) = 0 \tag{10}$$

which can be rearranged to give:

$$X_f = \frac{1}{H_f}\left[h_{le} - h_{lf} + \frac{1}{2}\left(v_e^2 - v_f^2\right)\right] \tag{11}$$

Having calculated the vapour quality X_f from the above equation, the density of the two-phase mixture at the end of the flashing stage, ρ_f, is then calculated from Equation (4), using the values of the liquid and vapour densities (ρ_{lf} and ρ_{vf}) given in Table 4. Finally, the cross-sectional area of the jet at the end of flashing, A_f, is obtained from conservation of mass (Equation 3), which can be rearranged to give:

$$A_f = \frac{\rho_e v_e A_e}{\rho_f v_f} \tag{12}$$

A summary of the calculated conditions at the end of flashing is given below in Table 5.

Table 5 Summary of calculated conditions at the end of the flashing stage

		DT1	DT2	DT4	SI Units
Cross-sectional area of pipe exit	A_e	0.00515	0.00701	0.00701	m^2
Velocity of ammonia liquid at pipe exit	v_e	25.5	27.3	25.5	m/s
Velocity of two-phase ammonia mixture at end of flashing stage	v_f	84.7	89.0	96.2	m/s
Quality at the end of the flashing stage (i.e., ammonia vapor mass fraction)	X_f	0.188	0.183	0.197	
Density of the two-phase mixture at the end of the flashing stage	ρ_f	4.26	4.38	4.05	kg/m^3
Cross-sectional area of the two-phase jet at the end of the flashing stage	A_f	0.222	0.300	0.277	m^2
Diameter of the jet at the end of the flashing stage	D_f	0.531	0.618	0.594	m

Stage 2 Air entrainment and evaporation of ammonia aerosol droplets

In the second stage of two-phase jet model, air is entrained into the jet and the ammonia aerosol droplets evaporate. The end of the stage is defined as the point where all of the droplets have evaporated. The amount of air entrained is determined to be just sufficient to evaporate all the droplets. It is assumed that the flow is in homogeneous equilibrium and there is zero slip between the phases, i.e., the droplets and vapor share both the same temperature and the same velocity. CERC (2000) gave the conservation equations for this stage of the calculation as follows:

Conservation of enthalpy

$$\alpha_{gj} M_g \Delta h_g + (1 - \alpha_{gj}) M_a \Delta h_a = 0 \tag{13}$$

Conservation of momentum

$$\rho_j v_j^2 A_j = \rho_f v_f^2 A_f \tag{14}$$

Conservation of mass

$$\frac{\rho_j v_j A_j}{A_f} - \rho_f v_f \left\{1 + \left[\frac{(1 - \alpha_g)}{\alpha_g}\right] \frac{M_a}{M_g}\right\} = 0 \tag{15}$$

where subscripts g and a refer to the contaminant gas (i.e., ammonia) and air, respectively. Subscript j refers to conditions at the end of the evaporation stage. The term α_{gj} is the mole fraction of ammonia at the end of the evaporation stage and the terms M_g and M_a are the relative molecular masses of ammonia and air (17.0305 g/mol and 28.97 g/mol, respectively).

Conservation of enthalpy

The equation for the conservation of enthalpy (Equation 13) expresses the following sum of terms:

Enthalpy at end of evaporation stage	=	Enthalpy at end of flashing stage	+	Enthalpy of entrained air

which can be written:

$$h_{gvj}\alpha_{gj}M_g + h_{aj}(1-\alpha_{gj})M_a = h_{gf}\alpha_{gj}M_g + h_a(1-\alpha_{gj})M_a \tag{16}$$

The two terms on the left-hand-side of the above expression are the enthalpy of ammonia vapour and the enthalpy of the air at the end of the evaporation stage. The molecular weights $M_g$and M_a appear in this equation because the specific enthalpies are mass based, but the fraction α_{gj} is molar based. In the above equation, h_{gvj} is the specific enthalpy of ammonia at the end of the evaporation stage (where the jet is all vapor) and h_{gf} is the specific enthalpy of ammonia at the end of the flashing stage (where the jet comprises both ammonia liquid and vapor). h_{aj} is the specific enthalpy of air at temperature T_j, and h_a is the specific enthalpy of air at the ambient air temperature T_a. Rearranging the above gives:

$$\alpha_{gj}M_g\left(h_{gf}-h_{gvj}\right) + (1-\alpha_{gj})M_a\left(h_a-h_{aj}\right) = 0 \tag{17}$$

which is the form given in the SMEDIS report (Equation 13) with $\Delta h_g = \left(h_{gf}-h_{gj}\right)$ and $\Delta h_a = \left(h_a-h_{aj}\right)$.

The enthalpy of ammonia (liquid and vapour) at the end of the flashing stage is:

$$h_{gf} = X_f h_{gvf} + \left(1-X_f\right)h_{glf} \tag{18}$$

where subscripts v and l refer to vapour and liquid phases and X_f is the quality (i.e., the ammonia vapour mass fraction). The above expression can also be written:

$$h_{gf} = h_{gvf} - \left(1-X_f\right)H_f \tag{19}$$

where, by definition, $H_f = h_{gvf} - h_{glf}$. Conservation of enthalpy can therefore be written:

$$\alpha_{gj}M_g\left[h_{gvf}-h_{gvj}-\left(1-X_f\right)H_f\right] + (1-\alpha_{gj})M_a\left(h_a-h_{aj}\right) = 0 \tag{20}$$

Assuming constant specific heats for ammonia vapor and air, C_{pgv} and C_{pa}, in the following expressions:

$$h_{gvf}-h_{gvj} = C_{p,gv}\left(T_f-T_j\right) \tag{21}$$

$$h_a-h_{aj} = C_{p,a}\left(T_a-T_j\right) \tag{22}$$

then the conservation of enthalpy equation becomes:

$$\alpha_{gj}M_g\left[C_{p,gv}\left(T_f-T_j\right)-\left(1-X_f\right)H_f\right] + (1-\alpha_{gj})M_a C_{p,a}\left(T_a-T_j\right) = 0 \tag{23}$$

It is assumed that the temperature is in equilibrium with the partial vapor pressure throughout this evaporation stage and the ammonia vapor mole fraction is given by:

$$\alpha_{gj} = \frac{P_{sat,gj}}{P_a} \tag{24}$$

where $P_{sat,gj}$ is the saturation vapor pressure from the Antoine equation:

$$\log_{10}\left(P_{sat,gj}\right) = a - \frac{b}{T_j + c} \tag{25}$$

with the coefficients a, b and c taken from the NIST Webbook, as described earlier.

Conservation of mass

The equation for the conservation of mass (Equation 15) is derived from the following expression:

Mass flow rate at the end of evaporation	=	Mass flow rate at the end of flashing	+	Mass flow rate of entrained air

The mass flow rate at the end of the evaporation stage is $\rho_j v_j A_j$, which includes contributions from both the ammonia mass and entrained air mass. The mass flow rate at the end of flashing is $\rho_f v_f A_f$, which includes contributions from ammonia vapor and liquid (but no air). The mass flow rate of entrained air is determined by scaling the mass flow rate $\rho_f v_f A_f$ by the ratio of the mass flow rate of air to the mass flow rate of ammonia, $\dot{m}_a/\dot{m}_g$, i.e.:

$$\rho_j v_j A_j = \rho_f v_f A_f + \rho_f v_f A_f \frac{\dot{m}_a}{\dot{m}_g} \tag{26}$$

This ratio $\dot{m}_a/\dot{m}_g$ is found from the ammonia vapor mole fraction at the end of the evaporation stage, α_{gj}, and the relative molecular masses of ammonia and air, M_g and M_a, as follows:

$$\frac{\dot{m}_a}{\dot{m}_g} = \frac{\left(1 - \alpha_{gj}\right) M_a}{\alpha_{gj} M_g} \tag{27}$$

The above expression can be derived by considering that the mole fraction α_{gj} is the number of moles of ammonia vapor to the total number of moles of ammonia vapor and air, and that the relative molecular mass equates to ratio of the mass of that substance to the number of moles. Substituting the above expression into the mass conservation equation and rearranging gives the equation for the conservation of mass given earlier by CERC (2000), i.e., Equation (15).

Density of ammonia vapor and air mixture at the end of evaporation

CERC (2000) gave the following expression for the density of the ammonia vapour and air mixture at the end of the evaporation stage:

$$\rho_j = \frac{\alpha_{gj}M_g + (1-\alpha_{gj})M_a}{\frac{\alpha_{gj}M_g}{\rho_{gj}} + \frac{(1-\alpha_{gj})M_a}{\rho_{aj}}} \tag{28}$$

where the contaminant gas (i.e., ammonia) and air densities, ρ_{gj} and ρ_{aj}, are evaluated at the temperature and pressure at the end of the evaporation stage, i.e., at temperature T_j and atmospheric pressure, P_a.

The above equation can be derived by considering that the density, ρ_j, is the ratio of the total mass to the total volume:

$$\rho_j = \frac{m_g + m_a}{V_g + V_a} \tag{29}$$

where the V is the volume, and from now on, the subscript j is dropped to simplify the equations, on the understanding that conditions are all evaluated at the end of the evaporation zone. The above equation can also be written:

$$\rho_j = \frac{m_g + m_a}{\frac{m_g}{\rho_g} + \frac{m_a}{\rho_a}} \tag{30}$$

The molar fraction of contaminant, α_g, multiplied by the molecular mass of contaminant, M_g, is:

$$\alpha_g M_g = \frac{n_g}{(n_g + n_a)}\frac{m_g}{n_g} = \frac{m_g}{(n_g + n_a)} \tag{31}$$

where n is the number of moles. Similarly:

$$(1-\alpha_g)M_a = \frac{(n_g + n_a - n_g)}{(n_g + n_a)}\frac{m_a}{n_a} = \frac{m_a}{(n_g + n_a)} \tag{32}$$

Substituting Equations (31) and (32) into (30) and rearranging gives the original expression from CERC (2000), i.e., Equation (28).

Solution of Enthalpy, Momentum and Mass Equations

The system of equations described above for conservation of enthalpy, momentum and mass are solved as follows:

1. The enthalpy equation:

$$\alpha_{gj} M_g \left[C_{p,gv} \left(T_f - T_j \right) - \left(1 - X_f \right) H_f \right] + \left(1 - \alpha_{gj} \right) M_a C_{p,a} \left(T_a - T_j \right) = 0 \qquad (33)$$

   is solved by iterating on temperature T_j until the left-hand-side of the above equation falls to zero. Note that the unknown molar fraction, α_{gj}, is a function of T_j, see Equations (24) and (25). The inputs (T_f, X_f and H_f) are given in Tables 4 and 5, the relative molecular masses M_g and M_a are given earlier, and values of the specific heats $C_{p,gv}$ and $C_{p,a}$ can be found in the NIST Webbook and other online sources, as summarised in Table 6. In the present work, the "goal seek" function in Microsoft Excel was used to iteratively solve Equation (33). An alternative method would be to input a range of values of T_j into the left-hand-side of Equation (33) and search through the results to find the value of T_j where the left-hand-side of Equation (33) falls to zero.

2. The equation for the density at the end of the evaporation stage (Equation 28) is solved to find ρ_j. The densities of ammonia vapor and air, ρ_{gj} and ρ_{aj}, are calculated from the ideal gas equation at the atmospheric pressure, P_a, and temperature, T_j.

3. There are two remaining unknowns, the velocity $\left(v_j \right)$ and area $\left(A_j \right)$, and two equations:
    a. conservation of mass:

$$\rho_j v_j A_j = \rho_f v_f A_f + \frac{\rho_f v_f A_f \left(1 - \alpha_{gj} \right) M_a}{\alpha_{gj} M_g} \qquad (34)$$

    b. and conservation of momentum:

$$\rho_j v_j^2 A_j = \rho_f v_f^2 A_f \qquad (35)$$

   Substituting one into the other gives:

$$v_j = \frac{\rho_f v_f^2 A_f}{\left[\rho_f v_f A_f + \frac{\rho_f v_f A_f \left(1 - \alpha_{gj} \right) M_a}{\alpha_{gj} M_g} \right]} \qquad (36)$$

   which can be simplified to:

$$v_j = \frac{v_f}{\left[1 + \frac{\left(1 - \alpha_{gj} \right) M_a}{\alpha_{gj} M_g} \right]} \qquad (37)$$

   The above equation is solved to find the velocity at the end of the jet mixing zone, v_j.

4. Finally, the area of the mixing zone is found from conservation of momentum:

$$A_j = \frac{\rho_f v_f^2 A_f}{\rho_j v_j^2} \tag{38}$$

5. The SMEDIS database defined the equivalent source area for the Desert Tortoise trials as a rectangular window with height equal to the half-width, W_j (see Figure 2), so the half-width of the source at the end of the evaporation stage, W_j, is found from:

$$W_j = \sqrt{\frac{A_j}{2}} \tag{39}$$

The results obtained from solving the enthalpy, momentum and mass equations are summarized in Table 6.

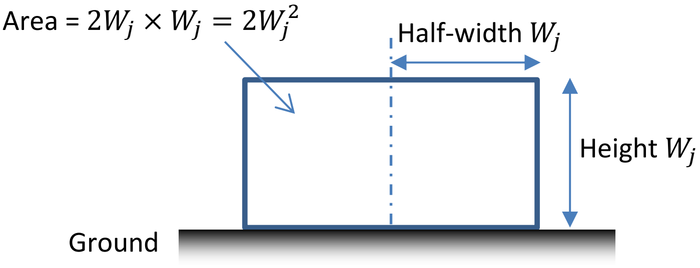

Figure 2 Shape of the equivalent source for the Desert Tortoise trials

Table 6 Summary of values from solution of enthalpy, momentum and mass equations in Stage 2

		DT1	DT2	DT4	SI Units
Specific heat at constant pressure for ammonia vapor	$C_{p,gv}$	2272.20	2272.40	2270.90	J/kg K
Specific heat at constant pressure for air	$C_{p,a}$	1005	1005	1005	J/kg K
Temperature at the end of the evaporation stage	T_j	204.67	204.78	205.07	K
Mole fraction of ammonia vapor at the end of the evaporation stage	α_{gj}	0.138	0.139	0.143	
Density of ammonia vapor at the end of the evaporation stage	ρ_{gvj}	0.910	0.910	0.902	kg/m^3
Density of air at the end of the evaporation stage	ρ_{aj}	1.548	1.548	1.534	kg/m^3
Density of the ammonia vapor and air mixture at the end of the evaporation stage	ρ_j	1.460	1.460	1.444	kg/m^3
Velocity at the end of the evaporation stage	v_j	7.27	7.70	8.59	m/s
Cross-sectional area of the jet at the end of the evaporation stage	A_j	87.8	120.3	97.6	m^2
Half-width of the source at the end of the evaporation stage	W_j	6.63	7.76	6.99	m

Distance to equivalent vapor-only source

As noted by CERC (2000), the conservation equations for enthalpy, momentum and mass do not involve any explicit calculation of the rate of air entrainment, so the distance to the end of the evaporation stage was not obtained in the previous calculations. To determine this distance, CERC (2000) suggested that a model such as EJECT (Tickle *et al.*, 1998) could be used in conjunction with the Ricou-Spalding entrainment assumption. However, details were not provided of the actual method used to determine the downstream distance of the vapor-only equivalent source in the SMEDIS database.

In the present work, the analytical jet model of Webber and Kukkonen (1990) with the Morton, Taylor and Turner (1956) entrainment model has been used to calculate the distance to the equivalent vapor-only source. A short description of this model can be found in the Lees Loss Prevention book (Lees, 2012). The model starts by defining ϕ as the ratio of the density of the jet to density of the surrounding air at the end of the evaporation stage:

$$\phi = \frac{\rho_j(T_j)}{\rho_a(T_a)} \tag{40}$$

where the density of the jet ρ_j is determined at the temperature T_j and the density of the surrounding air ρ_a at the ambient air temperature T_a.

The buoyancy flux B is then calculated from:

$$B = (\phi - 1) v_j A_j \tag{41}$$

and the momentum flux f from:

$$f = \phi v_j^2 A_j \tag{42}$$

The length scale L is calculated from:

$$L = \left(\frac{B^2}{\pi f}\right)^{1/2} \tag{43}$$

and the velocity scale U from:

$$U = \frac{f}{B} \tag{44}$$

The dimensionless variable p is calculated from:

$$p = \left(\frac{v_j}{U}\right)^{1/2} \tag{45}$$

and the dimensionless variable q from:

$$q = \left(\frac{1}{p^2} - 1\right)^{1/2} \tag{46}$$

It is assumed that the entrainment rate of fresh air is proportional to the velocity of the jet, with the constant of proportionality k taken here to be equal to 0.08. For further background on the choice of this entrainment coefficient, see Ricou and Spalding (1961) and Wheatley (1987).

Webber and Kukkonen (1990) obtained the following relationship between the quantity $(2kx/L)$ and the dimensionless variable q:

$$2kx/L = q(1 + q^2)^{1/2} + \ln\left[q + (1 + q^2)^{1/2}\right] \tag{47}$$

The distance downwind to equivalent vapor-only jet source, x_j, is then obtained from the length scale L and the assumed entrainment rate k as follows:

$$x_j = (2kx/L)\frac{L}{2k} \tag{48}$$

where $(2kx/L)$ in the above equation is obtained from Equation (47).

The results of these calculations for the Desert Tortoise trials are summarised in Table 7. An Excel spreadsheet with the calculations presented here is also available (file: “Equivalent source calc v1.2.xlsx”).

Table 7 Summary of calculated values used to determine the distance to the equivalent vapor-only source

		DT1	**DT2**	**DT4**	SI Units
Ratio of the densities of the jet to the air	ϕ	1.39	1.40	1.40	
Buoyancy flux	B	250.0	368.3	337.2	m^3/s
Momentum flux	f	6461	9970	10093	m^4/s^2
Length scale	L	1.75	2.08	1.89	m
Velocity scale	U	25.85	27.07	29.94	m/s
Dimensionless parameter	p	0.530	0.533	0.536	
Dimensionless parameter	q	1.60	1.59	1.58	
Calculated quantity	$(2kx/L)$	4.26	4.22	4.18	
Distance to equivalent vapor-only source	x_j	46.7	54.8	49.5	m

Nomenclature

a	Coefficient in Antoine equation
A	Jet cross-sectional area
b	Coefficient in Antoine equation
B	Buoyancy flux
c	Coefficient in Antoine equation
f	Momentum flux
h	Specific enthalpy
H	Heat of vaporization
k	Jet entrainment rate coefficient
L	Length scale
$\dot{m}$	Mass flow rate
M	Relative molecular mass
n	Number of moles
p	Dimensionless parameter in Webber and Kukkonen (1990) model
P	Pressure
q	Dimensionless parameter in Webber and Kukkonen (1990) model
T	Temperature
U	Velocity scale
v	Velocity
V	Volume
W	Half-width of the rectangular source area
x	Distance downwind
X	Quality, i.e. the mass fraction of vapor
α	Mole fraction of ammonia
ρ	Density
ϕ	Ratio of the jet density to the surrounding air density

Subscripts

a	Air component
e	Nozzle exit conditions
f	Conditions at the end of flashing (i.e., at the end of Stage 1)
g	Contaminant gas (i.e., ammonia) component
j	Conditions at the end of evaporation (i.e., at the end of Stage 2)
l	Liquid
v	Vapor

References

Carissimo B., Jagger S.F., Daish N.C., Halford A., Selmoer-Olsen S., Riikonen K., Perroux J.M., Wurtz J., Bartzis J.G., Duijm N.J., Ham K., Schatzmann M., Hall R. (2001) The SMEDIS database and validation exercise. International Journal of Environment and Pollution. 16 (1-6), p614-629. https://admlc.files.wordpress.com/2020/12/ijep_smedis_2001.pdf

CERC (2000) SMEDIS Model Evaluation Protocol, Report SMEDIS/96/8/D, Version 2.0, Cambridge Environmental Research Consultants Ltd (CERC), 7 December 2000. https://admlc.com/smedis-dataset/

Lees (2012) Lees' Loss Prevention in the Process Industries, Sam Mannan (Ed.), Fourth Edition, Butterworth-Heinemann, ISBN 978-0-12-397189-0.

Morton B.R., Taylor G.T. and Turner J.S. (1956) Turbulent gravitational convection from maintained and instantaneous sources, Proceedings of the Royal Society A, 234(1196), p1-24. https://doi.org/10.1098/rspa.1956.0011

Osborne N.S. and Van Dusen M.S. (1917) Latent heat of vaporization of ammonia, Bulletin of the Bureau of Standards, 14, p439-472. https://nvlpubs.nist.gov/nistpubs/bulletin/14/nbsbulletinv14n3p439_a2b.pdf

Ricou F.P. and Spalding D.B. (1961) Measurements of entrainment by axisymmetrical turbulent jets, Journal of Fluid Mechanics, 11 p21-32. https://doi.org/10.1017/S0022112061000834

Tickle G.A., Martin D. and Ramsdale S.A. (1998) EJECT – An integral model of a two-phase jet in a cross-flow, Theory manual for EJECT Version 2.01, Report AEAT-1517 Issue 2, AEA Technology, Warrington, UK, July 1998.

Webber D.M. and Kukkonen J.S. (1990) Modelling two-phase jets for hazard analysis, Journal of Hazardous Materials, 23(2) p167-182. https://doi.org/10.1016/0304-3894(90)85026-Y

Wheatley C.J. (1987) Discharge of liquid ammonia to moist atmospheres – survey of experimental data and model for estimating initial conditions for dispersion calculations, Safety and Reliability Directorate, Health and Safety Executive Report SRD/HSE/R410, April 1987. https://xnet.hsl.gov.uk/fileshare/public/3388/wheatley-srd-410-1987.pdf