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Modelling and Validation of Dispersion following an Instantaneous Release from a Pressurised Vessel

Henk W.M. Witlox*[a], Mike Harper[a], David Webber[b]

[a]DNV GL Software, Palace House, 3 Cathedral Street, London SE19DE, UK
[b]Integral Science and Software Ltd., 48a Warrington Road, Culcheth, Warrington, WA35RA
henk.witlox@dnvgl.com

This paper presents a new model for the initial dispersion phase of energetic instantaneous expansion following a catastrophic vessel rupture. This model has been implemented as a new sub-model in the Phast dispersion model UDM and is based on sounder physical principles than that included in the current release of Phast. The paper describes the analytical verification and validation of the new model for vapour releases and for two-phase releases without and with rainout. It is demonstrated that the new model agrees better with the available experimental data than the old model.

1. Introduction

Hazardous flammable and/or toxic materials are often stored in pressurised vessels. This paper deals with the modelling of the dispersion following a catastrophic rupture of the vessel leading to an instantaneous loss of containment. The Unified Dispersion Model (UDM) in the hazard assessment software package PHAST can account for two-phase jet, heavy and passive dispersion including droplet rainout and pool spreading/evaporation. The model can deal with a wide range of scenarios including both pressurised jet releases and unpressurised releases. As part of the current work the model has been improved for pressurised instantaneous releases. The new model includes an initial phase of energetic rapid expansion (modelled by a new UDM sub-model), and a subsequent phase of dispersion where equations are adopted applicable for unpressurised releases.

Witlox (2010) provides an overview of the UDM model in Phast including model verification and validation. A new version of the UDM has been developed for future inclusion in Phast, which includes improved modelling of time-varying dispersion including potential rainout using the so-called observer concept (Witlox and Harper, 2014).

The current UDM model in Phast includes a simplistic sub-model for the calculation of the initial dispersion phase of energetic expansion for pressurised instantaneous releases. The main limitations of this model are that this sub-model does not account for gravity effects, and that it presumes a single droplet size moving along a fixed upward angle resulting in too little rainout. Moreover droplets currently start at the edge of the cloud and therefore may erroneously rainout beyond the bund wall, if present.

Following the above a literature review has been carried out regarding both previous theoretical and experimental work. Amongst others this accounts for experimental work for ground-level pressurised releases for nitrogen vapour (Landis et al., 1994) and flashing liquid propylene (Maurer et al., 1977), and elevated flashing liquid releases for Freon 11 (Pettitt, 1990), Freon 12, propane and butane (Schmidli, 1993).

This paper first outlines the mathematical equations governing the new UDM sub-model called INEX. This model allows for both vapour and two-phase releases. In case of two-phase releases, the model accounts for droplet dispersion and potential time-varying droplet rainout to form a spreading evaporating liquid pool. Subsequently the paper describes the analytical verification of INEX for a number of specific cases. Finally it describes the validation of the model against experimental data for both cases of a pressurised vapour release and a pressurised two-phase release.

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2. New UDM sub-model (INEX)

Figure 1 depicts the subsequent dispersion phases during the initial UDM INEX stage of energetic expansion. The initial INEX state is based on discharge model results after isentropic expansion to ambient pressure and prior to air entrainment. The cloud is modelled as a sphere while elevated, as a truncated sphere during touching down and as a hemisphere after full touchdown. In case of a 2-phase release, the liquid droplets are assumed to be uniformly distributed throughout the cloud volume during the INEX expansion and thus travelling radially at a speed proportional to their distance from the cloud centre. Therefore rainout starts when the lower edge of the cloud hits the ground while it ends at full touchdown (see Figure 1). A transition from INEX to the standard UDM model is applied, when the INEX air entrainment reduces to the UDM air entrainment, or if the INEX spread rate reduces to the UDM gravity spreading rate. Any remaining liquid will rainout at this transition if the cloud is grounded, or possibly at a later stage (using standard UDM droplet modelling) if elevated.

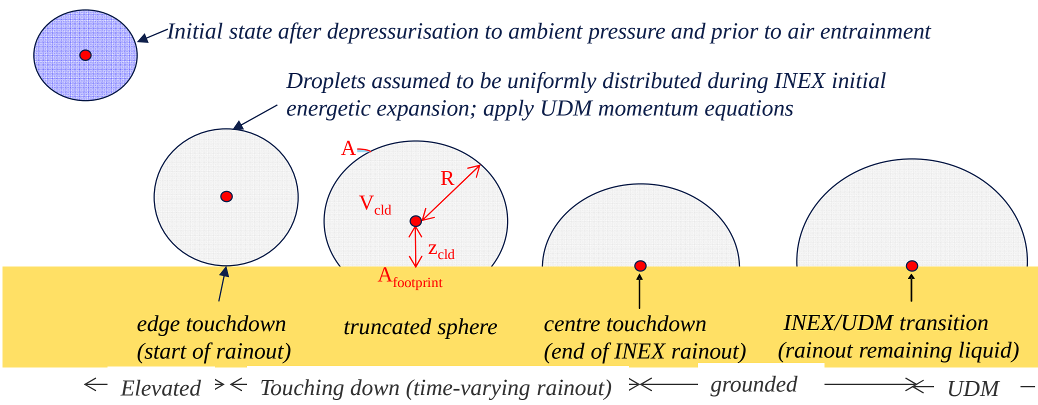


Figure 1: INEX dispersion phases for two-phase instantaneous release

From the above cloud geometry, the cloud volume V_{cld} can easily be expressed as a function of the cloud radius R and the cloud centre-line height z_{cld}. The INEX radial momentum (kg m/s) is defined as $I_r = m_{cld} U$. Here the radial cloud expansion speed U=dR/dt, and the total cloud mass $m_{cld} = m_{cL} + m_{cv} + m_{wa}$, where m_{cL} is the chemical liquid mass, m_{cv} the chemical vapour mass and m_{wa} is the mass of wet ambient air added to the cloud. The key INEX assumption is that the radial momentum is constant, apart from the loss of momentum due to rainout. Thus the following differential equations are applied in INEX for the radial momentum I_r, the entrained mass of wet air m_{wa}, and the rained out liquid mass m_{cL}^{ro},

$$\frac{dI_r}{dt} = -\frac{dm_{cl}^{ro}}{dt}U \tag{1}$$

$$\frac{dm_{wa}}{dt} = \rho_{wa}\frac{dV_{cld}}{dt} \tag{2}$$

$$\begin{aligned}\frac{dm_{cL}^{ro}(t)}{dt} &= 0 \ , \quad if \ z_{cld} \geq R(cloud\ elevated) \ or\ if\ z_{cld} = 0\,(cloud\ grounded) \\ &= \max\left\{K_D \frac{m_{cL}}{V_{cld}} A_{footprint}\left[\frac{z_{cld}}{R}U - \frac{dz_{cld}}{dt}\right], 0\right\}, \quad if\ 0 < z_{cld} < R\ \ (cloud\ touching\ down)\end{aligned} \tag{3}$$

Here t is the time (s), and the change in cloud volume is set as

$$\begin{aligned}\frac{dV_{cld}}{dt} &= AU \ , \qquad if\ z_{cld} \geq R(cloud\ elevated)\ or\ if\ z_{cld} = 0\,(cloud\ grounded) \\ &= AU + A_{footprint}\frac{dz_{cld}}{dt} \ , \quad if\ 0 < z_{cld} < R\ \ (cloud\ touching\ down)\end{aligned} \tag{4}$$

where A is the cloud surface area above the ground, and $A_{footprint}$ is the cloud footprint area (see Figure 1).

The first term in the right-hand side of rainout equation (3) represents the rainout due to cloud expansion and the second term represents the rainout due to the cloud centre-line height z_{cld} reducing. In the derivation of first term it is presumed that the radial cloud velocity linearly increases, and thus it can be derived that the vertical downward component at the footprint equals $(z_{cld}/R)\ U$. The maximum value of the parameter $K_D=1$, which presumes that all liquid hitting the ground will rainout.

The initial cloud speed $U(t=0)=U_o$ is set as $U_o=f_{kinetic}\ E_{exp}^{0.5}$. Here the specific expansion energy (J/kg) is set as $E_{exp} = h_{st} - h_f$, where h_{st} is the specific stagnation enthalpy and h_f is the specific final enthalpy after expansion to ambient pressure. Furthermore the fraction of total energy converted to kinetic energy is set to $f_{kinetic}=0.04$ following the recommendation of Pattison (1994) based on a best fit to data from Schmidli (1993).

In addition to the above equations, the standard UDM equations are applied during the INEX stage to evaluate the cloud centre location (from momentum equations including gravity effects), the cloud temperature, the cloud volume V_{cld} and the cloud phase distribution (from UDM two-phase thermodynamics equations). Following rainout, the model carries out pool spreading/evaporation calculations and the model accounts for pickup of vapour from the time-varying pool by the instantaneous cloud. For this purpose the so-called observer concept is applied to evaluate the time-varying dispersion in line with the paper by Witlox and Harper (2014).

3. Analytical solution for ground-level release

For a ground-level release, the INEX cloud is a hemisphere of radius R, and integration of Eq. (2) yields

$$m_{wa} = \rho_{wa}\left(V_{cld} - V_0\right) = \rho_{wa}\frac{2\pi}{3}\left(R^3 - R_o^{\ 3}\right) \tag{5}$$

where R_o is the initial cloud radius (following depressurisation to ambient and prior to air entrainment). In case of a two-phase ground-level release, it is presumed that 50% of the liquid rains out immediately, while the remaining liquid moves out radially in upward directions. Therefore according to Eq. (1) radial momentum $I_r = m_{cld}U$ is constant and therefore [m_o = released vessel mass after immediate rainout]:

$$m_o U_o \approx m_{cld} U \approx \left[m_0 + m_{wa}\right]\frac{dR}{dt} = \left[m_0 + \rho_{wa}\frac{2\pi}{3}\left(R^3 - R_o^{\ 3}\right)\right]\frac{dR}{dt} \tag{6}$$

By means of separation of variables R and t, the above equation can be integrated to yield,

$$t = \frac{R}{U_o}\left\{1 + \left[\frac{\rho_{wa}}{\rho_o}\right]\left[\frac{1}{4}\left(\frac{R}{R_o}\right)^3 - 1\right]\right\} - \frac{R_0}{U_o}\left\{1 - \frac{3}{4}\left[\frac{\rho_{wa}}{\rho_o}\right]\right\}, \quad U = \frac{U_o}{1 + \left[\frac{\rho_{wa}}{\rho_o}\right]\left[\left(\frac{R}{R_o}\right)^3 - 1\right]} \tag{7}$$

where $\rho_o = m_o/(2\pi R_o^3/3)$ is the initial chemical density after the initial immediate rainout. Thus the above expression is used to analytically evaluate cloud radius R and cloud expansion speed U versus time t.

4. Model verification and validation

4.1 Ground-level nitrogen vapour releases (Landis et al.)

Landis et al. (1994) carried out experiments involving an instantaneous release of nitrogen vapour from a cylindrical tank (length 12”, radius 2”) with a range of stagnation temperatures (273 or 303K) and pressures (4.2, 8.2, 21.5 and 71.7 bara). These experiments have been modelled as hemispherical grounded releases.

Figure 2 plots the dimensionless cloud volume versus a dimensionless time, where the INEX numerical predictions are chosen to correspond to the experiment with 273K and 71.7bara. The plot confirms perfect matching of the above analytical solution against the new INEX numerical model. The new INEX model slightly over-predicts the data, while the old INEX model significantly under-predicts. In this context note that the old INEX radius R is always set presuming a sphere (including grounded releases), and therefore its initial radius R_o is a factor $2^{-1/3}$ smaller than the new INEX hemispherical radius.

The plot also includes results from the model by Landis et al. (1994), who presume frontal capture of the cylindrical tank (for setting air entrainment) in conjunction with a hemispherical assumption (the corresponding figure 5 in their paper appears to show an incorrect curve). This differs from our assumption of air entrainment across the entire hemispherical cloud surface area A. Neither do they report initial values ρ_o, R_o or U_o and this could also partially account for difference of our model with the data.

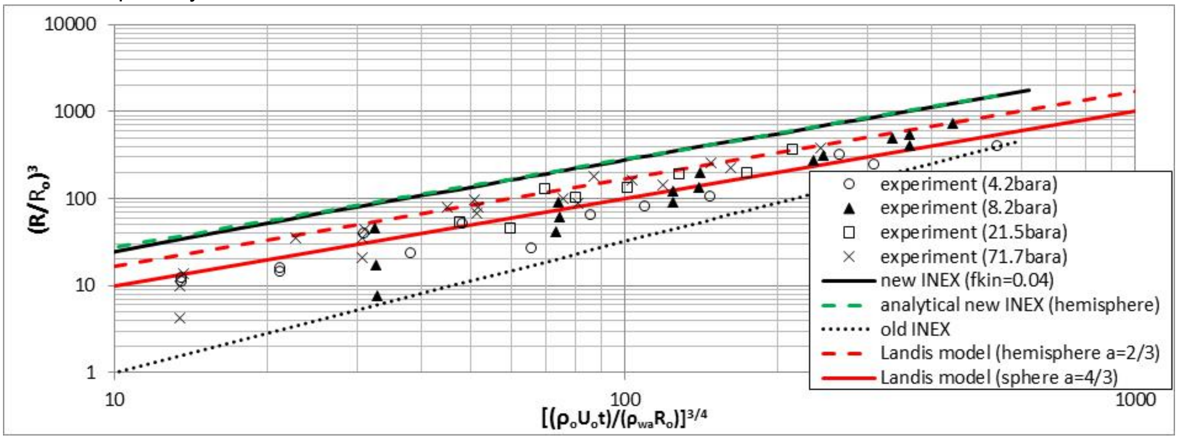
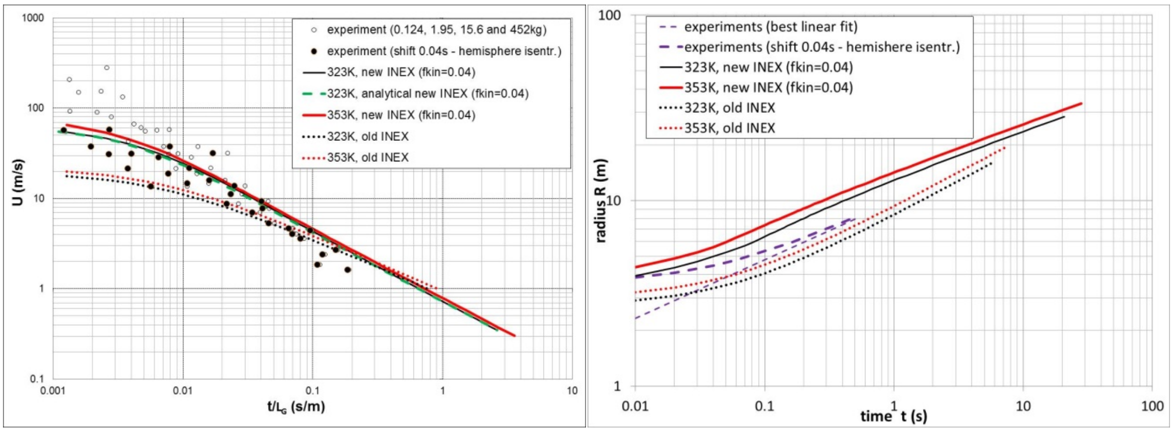


Figure 2: Validation of cloud volume versus time against Landis nitrogen experiments

4.2 Ground-level flashing propylene liquid releases (Maurer et al.)

Maurer et al. (1977) carried out experiments involving an instantaneous release of heated flashing propylene liquid from a cylindrical tank with stagnation pressure 60barg, stagnation temperature 323 or 353 K, and considering a range of tank sizes (release masses 0.125, 0.42, 1.95, 6.55, 15.6 or 452kg). These experiments have been modelled as hemispherical grounded releases.



(a) speed versus scaled time *(b) radius versus time*

Figure 3: Validation against Maurer experiment (propylene, 452kg, 60barg, 323K or 353K)

Maurer adopts a 'normalised' time t/L_G (s/m) where L_G is the cube root of the volume (V_G) of twice the released mass (2M) of propylene in the gaseous phase at 0 Celsius and 1bar. For the case of M=452kg (tank length 2.8m, tank diameter 0.7m), Figure 3a plots the cloud speed U versus t/L_G, where L_G=7.83m. Figure 3b plots the radius R versus time t. The INEX model starts from time t=0 after the initial isentropic expansion to atmospheric pressure, and (by comparing experimental radii with initial INEX radius) this is ~ 0.04s after the start of the release. Therefore we have shown in both plots experimental data obtained from Maurer's paper, both with and without a time shift of 0.04s. The plot again confirms perfect matching of the analytical solution with the new INEX numerical predictions. The new INEX model closely agrees with the data, and appears to slightly over-predict. The old INEX model under-predicts for smaller times and more closely agrees with the data for the visible cloud at larger times.

4.3 Elevated flashing Freon liquid releases (Pettit)

Following earlier PhD's at South Bank University, Pettitt (1990) carried out experiments involving a catastrophic failure of a 1 litre elevated glass sphere by hammer impact. The glass sphere was elevated at 0.25m height and filled with a saturated liquid. A range of experiments was carried out including variation of material (Freon 11, 113 or 114), % fill, and stagnation pressure. The conditions were chosen such as to avoid

rainout. In line with our model assumptions, he confirmed the cloud increases as a sphere, with expansion speed U decreasing with time and with droplet speeds independent of size and moving in radial directions.
Figure 4 includes INEX validation results of cloud speed U versus cloud radius R against experimental data for a 1 litre vessel with a 100% fill of Freon 11 and stagnation pressure of 4.10barg. Experimental data include minimum, mean and maximum values. It is seen that the old INEX model significantly under-predicts, while the new INEX model slightly under-predicts. The figure also includes the result from an additional new INEX run, where a value of the fraction of total energy converted to kinetic energy, $f_{kinetic}$=0.15, is applied such that the INEX speed matches the observed data at the initial INEX radius (after isentropic expansion to ambient pressure). It is seen that this results in improved agreement against the experimental data.

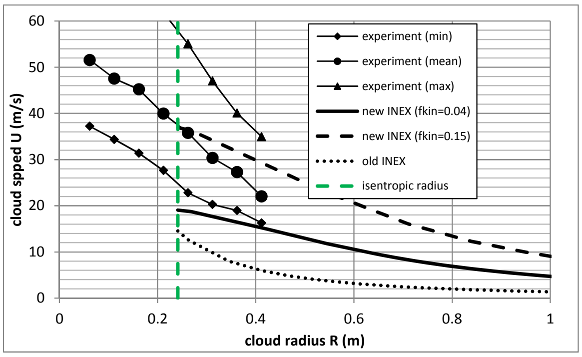
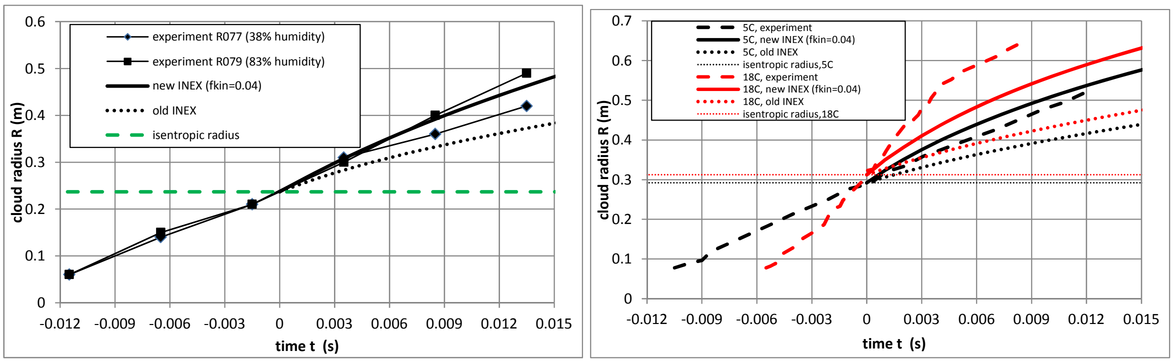


Figure 4: Cloud speed validation against Pettitt experiments (Freon 11, 100% fill, 4.10 barg, 1 litre)

Validation of cloud speed U was also carried out against Freon 11 experiments with 50% fill and pressures ranging between 1.4 and 5.7barg, and similar conclusions were derived as above.

4.4 Elevated flashing Freon, propane and butane liquid releases (Schmidli)

As part of a PhD at the Swiss Federal Institute of Technology, Schmidli (1993) carried out similar experiments to Pettitt. He considered a range of flask sizes (0.1, 1 or 1 litre), materials (R-114, R-12, propane and butane) and superheats. His experiments included both grounded and elevated releases, and unlike Pettitt he also investigated effects of rainout.



(a) R-12, 1 litre, 22C, 0.62m elevation (b) propane, 2 litre, 5 or 18C, 1m elevation

Figure 5: Cloud radius versus time for Schmidli experiments (100% fill)

Figure 5 includes INEX predictions against experimental data for R-12 (stagnation temperature 22C corresponding to 52.1C superheat and saturated stagnation pressure 6 bara, ambient humidity 38 or 83%) and propane (5C or 18C corresponding to 47.4C and 60.4C superheat and pressures of 5.52 and 7.94bara). Again experimental data are shifted such that at time t=0 the INEX isentropic radius is reached.
For R-12 the visible aerosol cloud radius slightly increased with humidity, while the effect of humidity on INEX predictions is insignificant. New INEX predictions of cloud radius are larger than those of the old INEX and closer to the experimental data. For propane the effect of superheat appears to be larger for the experiments than for the new model, but this may result from increased condensation of the water in the moist air, and hence a more visible cloud.

5. Conclusions

A new model (INEX) has been formulated for the initial dispersion phase of initial energetic expansion following a pressurized instantaneous release. For ground-level vapour or two-phase releases the correctness of the numerical predictions has been confirmed against an analytical solution.

INEX is based on more sound physical principles than the previous model. Overall the old model tends to under-predict the cloud radius and cloud speed versus time, while the new model provides larger predictions and more closely agrees against experimental data. Therefore the new model produces smaller concentrations and doses, and is less conservative.

Experiments identified so far derive the cloud radius and cloud speed from the visible cloud front. Additional experimental work to measure concentrations would provide a sounder basis for model validation. As part of future work it is planned to carry out validation of the new model against rainout data.

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References

Landis J.G., Linney R.E, Hanley B.F., 1994, Dispersion of instantaneous jets, Process Safety Progress 13 (1), 35-40

Maurer B., Schneider H., Hess K., Leuckel W., 1977, Modelling of vapour cloud dispersion and deflagration after bursting of tanks filled with liquefied Gas, Int. Loss Prevention Symposium, Heidelberg

Pattison M.J., 1994, E.C. Cloud Project – Initial stages of release, Draft note, Department of Chemical Engineering and Chemical Technology, Imperial College, London

Pettitt G.N., 1990, Characterisation of two-phase releases, PhD Thesis, South Bank Polytechnic, London

Schmidli J., 1993, The initial phase of sudden releases of superheated liquid, Ph.D. Thesis, ETH, Zurich

Witlox H.W.M., 2010, Overview of consequence modelling in the hazard assessment package Phast, Paper 7.2, 6th AMS conference on applications of air pollution meteorology, Atlanta, USA, 17-21 January 2010

Witlox H.W.M, Harper M., 2014, Modelling of time-varying dispersion for releases including potential rainout, Process Safety Progress 33 (3), 265-273