



FLASHING LIQUID JETS AND TWO-PHASE DROPLET DISPERSION

Henk Witlox and Mike Harper, DNV Software, London, UK , www.dnvsoftware.com
Phil Bowen and Vincent Cleary, Cardiff University, UK

Abstract

Loss of containment often results in flashing releases of hazardous chemicals into the atmosphere. Rainout of these chemicals reduces airborne concentrations, but can also lead to extended cloud duration because of re-evaporation of the rained-out liquid. Therefore for hazard assessment one must use models which accurately predict both the amount of rainout and its rate of re-evaporation. However, the findings of a literature survey reveal weaknesses in the state-of-the-art for modelling the sub-processes of droplet atomisation, atmospheric expansion, two-phase dispersion, rainout, pool formation and re-evaporation. The current paper reports the results of implementations of recommendations from this survey, deriving from scaled water experiments droplet size correlations for conditions ranging from negative to high superheat. As a whole these correlations describe a tri-linear function of droplet size (expressed as Sauter mean diameter) as a function of superheat. This function describes the regimes of non-flashing, the transition between non-flashing and flashing, and fully flashing. The new correlations have been compared with previous correlations recommended by the Dutch Yellow Book and CCPS books. The correlations are validated against published experiments including the STEP experiments (flashing propane jets), experiments by the Von Karman Institute (flashing R134-A jets), and water and butane experiments carried out by Ecole des Mines and INERIS. The rainout calculations by the dispersion model have been validated against a subset of the CCPS experiments (flashing jets of water, CFC-11, chlorine, cyclohexane, monomethylamine).

Keywords: flashing liquid jets, droplet dispersion, rainout

1. Introduction

Many accidents involve two-phase flashing releases of hazardous chemicals into the atmosphere. Rainout of these chemicals results in reduced concentrations in the remaining cloud, but can also lead to extended cloud duration because of re-evaporation of the rained-out liquid. For accurate hazard assessment, one must accurately predict both the amount of rainout and re-evaporation of the cloud. Figure 1 illustrates the problem. After elevated two-phase discharge, evaporating droplets move away from the plume centre-line. If droplets reach the substrate, rainout occurs leading to the formation of a spreading liquid pool which provides a secondary source of vapour.

A 'Phase I' scoping project was carried out by Witlox and Bowen¹, which involved a detailed literature review on flashing liquid jets and two-phase droplet dispersion. This project was sponsored by DNV, the UK Health and Safety Executive, Exxon Mobil and ICI Eutech. The review considered models and validation data for the sub-processes of atomisation, atmospheric expansion to ambient pressure, two-phase dispersion, rainout, pool formation and re-evaporation. This project served to establish the state-of-the-art and provide recommendations for:

- Model for atmospheric expansion from orifice to ambient conditions (particularly for initial droplet size, isentropic versus isenthalpic expansions; post-expansion data are initial droplet size, flash fraction, velocity)
- Air entrainment for two-phase jet releases (including liquid droplets)
- Conservation equations for droplets downstream of the orifice (including droplet distribution)
- Rainout criteria (including cut-off for droplet size diameter)
- Re-evaporation from pool
- Other practical influences, e.g. orifice characteristics

It was found that the source term for the downstream dispersion calculations was ill-defined due to lack of a justifiable, validated atomisation model. No experiments were found to be available for releases with significant rainout, which would enable to link the initial post-expansion conditions with downstream rainout or airborne concentration. Only two models were found which attempt to model the primary two-phase processes on a physical basis, the DNV 'Unified Dispersion Model' UDM^{2,3} and its multi-compound generalisation by Mobil^{4,5}. Potential limitations of these models were discussed – further details may be found in Witlox and Bowen¹.

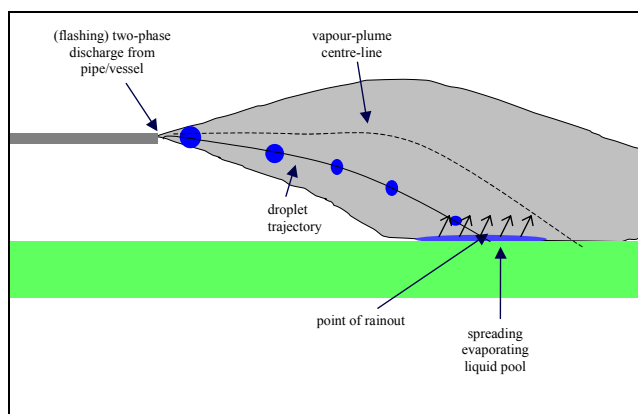


Figure 1. Droplet evaporation and rainout

A follow-up Phase II project^{6,7} funded by DNV, Atofina, Gaz De France and RIVM (Dutch government) was initiated to implement the recommendations from Phase I. It derived from scaled water experiments droplet size correlations for conditions ranging from low to high superheat. The current paper summarises the results of this project. It also includes considerable additional updates after Phase II, such as additional validation studies and updates to the original CCPS droplet correlation.

Section 2 reports the results of scaled experiments for water jets and the development of droplet-size correlations. Section 3 describes in detail this newly derived correlation as well as previous correlations recommended in the literature. Section 4 compares the different correlations and describes their validation against experimental data. In Section 5 rainout calculations are reported for CCPS experiments from a two-phase dispersion model using as input the initial droplet size from the above correlations. Section 5 discusses the necessity for further studies, and Section 6 summarises the main conclusions.

2. Scaled water experiments

The first stage of the Phase II work involved scaled experiments for 2-phase water jets. Using Phase Doppler

Anemometry, the experiments measured velocity and droplet size distributions as close to the orifice as possible (to represent post-expansion data) in order to derive an improved atomisation correlation valid for release conditions. Experiments were undertaken for both low superheat (non-flashing jets; mechanical break-up droplet size criterion) and significant superheat (flashing jets).

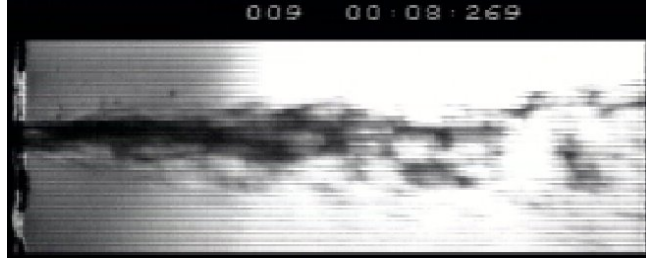
Depending on the initial thermodynamic state of a pressurised containment of a liquid, droplets in a two-phase jet can be formed primarily as a result of either aerodynamic (mechanical) break-up or flash atomisation. For sub-cooled jets, liquid jet break-up into droplets is dominated by competition between aerodynamic and surface tension forces at the liquid/gas interface. This process is commonly known as mechanical or aerodynamic break-up. Aerodynamic break-up occurs when any random protrusion on the surface of a jet is subjected to a lower gas pressure over its crest than its base. The faster the jet relative to the surrounding atmosphere, the more pronounced the effect. Eventually, this protrusion may detach from the jet to form a droplet, which may break up further until a stable size is reached⁸. Aerodynamic break-up is typically a feature of sub-cooled releases. 'Flashing' on the other hand, is a feature of superheated releases. In terms of the droplet size and therefore the potential hazard, the difference between break-up mechanisms is hugely significant.

As demonstrated in Figure 2, three different stages of transition are identified (corresponding to increasing superheat):

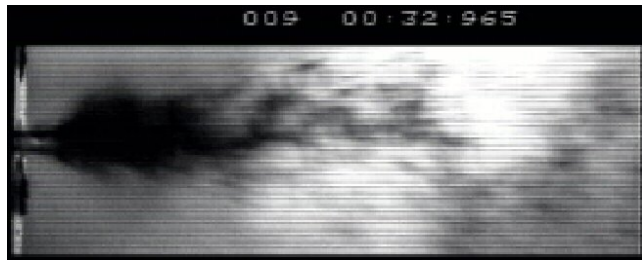
- (A) Condition A is characterised as the condition, at which external bubble nucleation first occurs. A significant liquid core remains immediately downstream of the exit orifice, before completely disintegrating further downstream to create a distinctive wide angled spray.
- (B) Condition B is characterised by an initial unbroken jet, which shatters suddenly and violently a short distance from the nozzle exit.
- (C) Condition C is characterised as the condition at which the core of the liquid jet violently disintegrates at the nozzle (with bubble nucleation inside the orifice).

The correlation derived as part of the experimental work is summarised in Section 3.3. This new correlation describes the regimes of non-flashing (before point A), the transition between non-flashing and flashing (between points A and C), and fully flashing (after point C). In addition to droplet size correlations for the Sauter Mean Diameter (SMD), the experimental work also derived correlations for droplet size distributions (around the SMD). The reader is referred to

the overall Phase II report⁶ for further details on the experiments and the derivation of the above correlations.



(A)



(B)



(C)

Figure 2. Transition stages between mechanical break-up and fully flashing

3. Overview of droplet size correlations

This section includes a description of two of the most commonly recommended correlations for the Sauter Mean Diameter (SMD) of the droplet size (CCPS and Yellow Book correlations), as well as a description of the newly proposed correlation. Witlox and Bowen¹, the CCPS RELEASE book⁹ and Ramsdale⁸ provide a wider list of correlations and a detailed review of these. The CCPS and Yellow Book droplet-size correlations are expressed in terms of post-expansion data, and therefore these very much depend on the adopted expansion equations; see 0 for a brief discussion.

3.1 Weber/CCPS correlation

This model is recommended in the CCPS book by Johnson and Woodward⁹ for predicting aerosol rainout in accidental

releases. The droplet size d_d (SMD) is set as the minimum of the droplet size d_{da} , derived from “mechanical or aerodynamic” break-up and the droplet size d_{df} derived “flashing” break-up,

$$d_d = \min \{ d_{da}, d_{df} \} \quad (1)$$

Here d_{da} is calculated as a function of the critical Weber number

$$d_{da} = \frac{\sigma_L We_{crit}}{u_f^2 \rho_a} \quad (2)$$

where u_f is the final post-expansion velocity (m/s), σ_L the post-expansion surface tension of the liquid (N/m), and ρ_a the atmospheric density (kg/m³); furthermore We_{crit} is the critical value of the gas Weber number, taken as 12.5 in line with recommendations by the Yellow book¹², Brown and York¹⁰ and Heinze¹¹.

Using the PHAST model UDM, Woodward calculated droplet diameters such as to best match observed rainout data for the CCPS rainout experiments. These “experimental” drop sizes were correlated against a number of differing parameters, of which partial expansion energy, E_p , was the most effective correlator for droplet size d_{df} . Thus d_{df} (m) is calculated as a function of E_p (J/kg)ⁱ

$$d_{df} = 0.833 * 10^{-3} - 0.0734 * 10^{-3} \ln(E_p) \quad (3)$$

with the partial expansion energy given by

$$E_p = -\Delta h - [P_v^{sat}(T_{st}) - P_a] v_{st} + [P_{st} - P_v^{sat}(T_{st})] v_{st}, P_a < P_v^{sat}(T_{st}) \quad (4)$$

$$= (P_{st} - P_a) v_{st}, P_v^{sat}(T_{st}) \leq P_a$$

where Δh is the change in material enthalpy from stagnation to final post-expansion conditions (J/kg), P_{st} the stagnation pressure (N/m²), T_{st} the stagnation temperature (K), v_{st} the stagnation specific volume, P_a the ambient pressure (N/m²), and P_v^{sat} the saturated vapour pressure. The two cases in the above equation correspond to superheated liquid (liquid-to-two-phase expansion) and sub-cooled liquid (liquid-to-liquid expansion), respectively. The flashing droplet correlation is derived from experiments involving releases from leaks only. Therefore its applicability to releases from pipes and to instantaneous releases is questionable. In the case of the release from a vessel (without attached pipe) and ‘meta-stable liquid’ assumption between the stagnation and the orifice conditions (i.e. no flashing within the orifice,

ⁱ This correlation is implemented in PHAST and slightly deviates from the correlation reported in the CCPS book.

$T=T_{st}$, $P=P_a$), the above droplet size formula should always be associated with an isentropic atmospheric expansion (conservation of mass, entropy, energy) in line with the assumption taken by Johnson and Woodward.

3.2 Appleton/Wheatley correlation recommended by Yellow-book

For finite-duration spray releases, the Yellow Book¹² recommends the initial droplet-size calculation method based on the work by Appleton¹³ and presented by Wheatley¹⁴. It is defined as follows:

$$d_d = 1.89 d_f \sqrt{1 + 3 \frac{We_{Lf}^{0.5}}{Re_{Lf}}}, \text{ if } \{We_{Lf} < 10^6 Re_{Lf}^{-0.45} \text{ and } T_o < 1.11 T_v^{sat}(P_a)\} \quad (5)$$

$$= \frac{\sigma_L We_{crit}}{u_f^2 \rho_a}, \text{ else}$$

where T_o is the exit (orifice) temperature (prior to the expansion); $T_v^{sat}(P_a)$ is the normal boiling temperature of the released component, i.e. the saturated temperature at ambient pressure. Here the liquid Reynolds number and the liquid Weber number correspond to the post-expansion state,

$$Re_{Lf} = \frac{\rho_L u_f d_f}{\mu_L}, \quad We_{Lf} = \frac{\rho_L u_f^2 d_f}{\sigma_L} \quad (6)$$

where u_f is the post-expansion velocity, d_f the post-expansion diameter, and with all material properties evaluated at the post-expansion temperature T_f . Note that the above equation actually represents two types of 'mechanical break-up' criteria. The second part of this criterion is identical to the Weber criterion (2) applied for the above Weber/CCPS correlation, however with $We_{crit} = 15$ applied instead of $We_{crit}=12.5$.

3.3 New correlation recommended by Phase II of current JIP

Mechanical break-up criterion

This criterion was derived from experimental data for sub-cooled jets⁶. The droplet SMD = d_{da} (m), using the mechanical (aerodynamic) break-up criterion, is calculated as a function of the ratio L/d_o , the orifice liquid Reynolds number Re_{Lo} and the orifice liquid Weber number We_{Lo} , as follows:

$$\frac{d_{da}}{d_o} = F(We_{Lo}, Re_{Lo}, \frac{L}{d_o}) = 64.73 We_{Lo}^{-0.533} Re_{Lo}^{-0.014} \left(\frac{L}{d_o}\right)^{0.11} \quad (7)$$

with

$$Re_{Lo} = \frac{\rho_L u_o d_o}{\mu_L}, \quad We_{Lo} = \frac{\rho_L u_o^2 d_o}{\sigma_L} \quad (8)$$

Here d_o is the orifice diameter, L the thickness of the vessel wall (case of release from hole in vessel) or pipe length (for release from pipe), σ_L the surface tension of the liquid (N/m), u_o the orifice velocity, ρ_L the liquid density (kg/m³), and μ_L the liquid dynamic viscosity (Pa s). Unlike the previous correlations, the above correlation is expressed as function of orifice data (prior to expansion to atmospheric pressure) and not in terms of final post-expansion data. The above expression is applied for $2 < L/d_o < 50$. For $L/d_o < 2$ and $L/d_o > 50$ the cut-off values of $L/d_o = 2$ and $L/d_o = 50$ are applied.

Transition criterion to flashing

This transition criterion was derived from experimental data for flashing jets⁶. Figure 3 plots the SMD d_d (m) as a trilinear function of superheat ΔT_{sh} ,

$$\Delta T_{sh} = T_o^u - T_v^{sat}(P_a) \quad (9)$$

Here T_o^u is the temperature immediately upstream of the orifice, and $T_v^{sat}(P_a)$ the saturated temperature at the ambient pressure P_a .

Prior to point A mechanical break-up applies, with the droplet size determined from Equation (7). Between points A and C transition to fully flashing occurs (see Figure 2). For the end point C of the transition the droplet SMD is assumed to have been reduced by a factor of 2.4 with respect to point A. Prior to point C the assumption of metastable liquid is assumed (liquid-to-liquid expansion from stagnation to orifice conditions; non-equilibrium). After point C fully flashing is assumed, with liquid to two-phase expansion from stagnation to orifice conditions (equilibrium). After point D the SMD is assumed to decrease slowly - nominally 0.1 $\mu\text{m}/\text{K}$.

The superheat at the start ($\Delta T_{sh} = \Delta T_{sh}^A$) and end ($\Delta T_{sh} = \Delta T_{sh}^C$) of the transition to flashing are set by determining ΔT_{sh} from the following criteria

$$\text{Start point A: } Ja \phi = 55 We_v^{-\frac{1}{7}}, \text{ with } \phi = 1 - e^{-2300 \left(\frac{\rho_v}{\rho_l}\right)} \quad (10)$$

$$\text{End point C: } Ja \phi = 150 We_v^{-\frac{1}{7}} \quad (11)$$

where ρ_v and ρ_l are the vapour and liquid density evaluated at the orifice temperature. In accordance with the paper by Kitumura¹⁵, the vapour Weber number We_v and the Jacob number Ja are evaluated as

$$We_v = \frac{\rho_v u_o^2 d_o}{\sigma_L}, \quad Ja = \frac{C_{pL} \Delta T_{sh} \rho_L}{h_{fg} \rho_v} \quad (12)$$

where C_{pL} is the specific heat of the liquid (J/kg/K), and h_{fg} the latent heat of evaporation (J/kg), both evaluated at the orifice temperature.

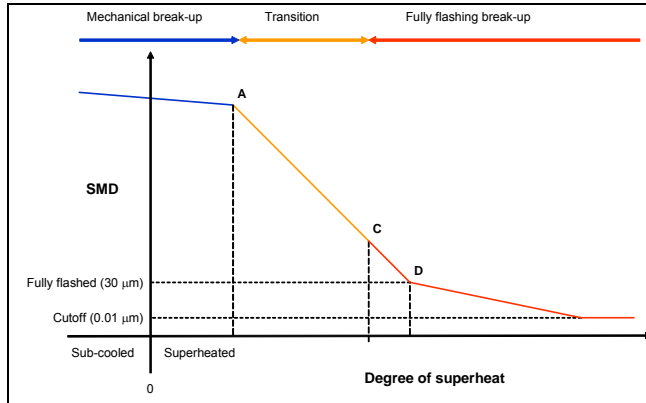


Figure 3. Tri-linear curve for Sauter Mean Diameter as function of superheat

4. Comparison and validation of droplet size correlations

The second stage of the Phase II work involved the implementation and further validation/testing of the above droplet size correlations, which have been carried out by further developing models in the DNV consequence modelling package PHAST. These models included the discharge model DISC and the atmospheric-expansion model ATEX and the new models are planned to be made available in a version of PHAST in the near future.

Model comparison for mechanical break-up

First the newly proposed mechanical break-up criterion was compared against the current CCPS and the Yellow-Book correlation (critical Weber-number correlations), as well as correlations proposed by Tilton and Farley¹⁶ and Elkotb¹⁷. Figure 4 presents a comparison between the SMD predictions for these correlations. It presents the influence of velocity at the orifice (prior to atmospheric expansion) against predicted SMD, for the specific cases of two nozzles of orifice diameter 1mm but with differing aspect ratios of 1.0 and 10. The velocity data presented in Figure 4 above 50 m/s are an extrapolation outside the experimental range of this work (stagnation pressures above 24 bar). Within the experimental range, the newly proposed correlation for this specific example results in smaller droplet sizes than the CCPS and Yellow-Book Weber-number correlations, and larger droplet sizes than those predicted by the Tilton and Farley and Elkotb correlations.

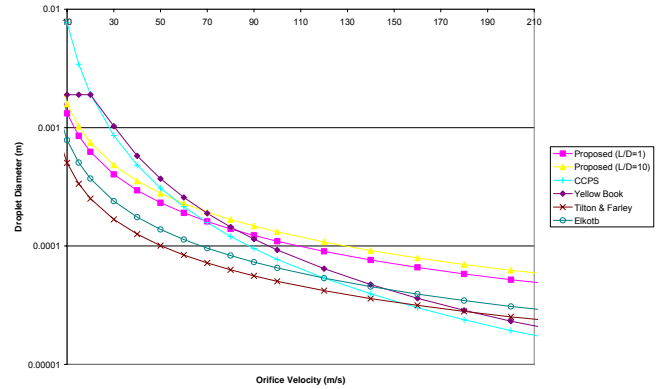


Figure 4. Comparison of correlations for mechanical break-up

Model validation for flashing jets

The above extended models have been validated against a range of experiments, i.e. STEP^{18,19} (flashing propane jets), VKI²⁰ (flashing R134-A jets), the above new Cardiff experiments (water)⁶, and experiments by Ecole des Mines (flashing water jets) and INERIS (flashing butane jets) as reported in the paper by Touil et al.²¹.

Table 1 summarises the experimental conditions, measurements and SMD predictions for these experiments. The input data in this table has been derived from the above papers; see Witlox et al.⁶ for details. For the Ecole-des-mines water experiments WA-OR1, WA-OR2 the second and third figures for the SMD are obtained from Bigot²²: the second figure is the SMD for the droplets with $D < 150 \mu\text{m}$, while the third figure is for the entire droplet population, including the few large droplets ($150 \mu\text{m} < D < 600 \mu\text{m}$).

The orifice velocity in Table 1 is calculated from the flow rate where available. Otherwise (in line with the observations in the Cardiff experiments) it is set using a discharge coefficient (C_d) of 0.75 (except for Cardiff 1 for which 0.7 was adopted). The table finally includes the SMD values for the three correlations discussed in the preceding section:

- Yellow Book SMD. As recommended in the Yellow Book this is based on final post-expansion conditions using the conservation of momentum model for atmospheric expansion from the orifice to the ambient pressure. However, to illustrate the difference, also included is the Yellow Book droplet size formula in conjunction with the isentropic model.
- CCPS flashing and CCPS mechanical break-up SMD. As recommended in the CCPS Book these are based on final post-expansion conditions from the isentropic model.
- JIP proposed SMD. This is expressed in terms of orifice data and is therefore independent of the post-orifice expansion calculations.

Experiment ⁱⁱ	STEP	VKI	Cardiff 1	Cardiff 2	BU-OR	WA-OR1	WA-OR2
<i>Experimental conditions</i>							
Material	Propane	R134-A	water	water	Butane	Water	Water
storage pressure (bar)	10.75	8.25	11.0	11.5	3	9.2	11.4
storage temperature (C)	29.8	23	155	155	23.85	164	167
Orifice diameter (mm)	5	1	1	0.75	5	2	2
L/d _o	07	07	3.4	4.53	0	0	0
ambient pressure (atm)	0.91	1	1	1	1	1	1
ambient temperature (C)	30	20?	20?	20?	23.85?	10	9
<i>Measurements</i>							
flow-rate (kg/s)	0.2	unknown	unknown	unknown	unknown	0.08	0.09
downstream location (mm)	95	187	250	250	200	200	200
post-expansion SMD (µm)	32.4	80-100	63	60	80	79, 67/350	61, 76/228
<i>Model predictions</i>							
orifice velocity (m/s)	20.87	26.0	32.75	35.96	19.72	28.13	31.75
Yellow Book SMD (µm)	531	286	680	564	487	888	694
Yel Book isentr. SMD(µm)	4.6	15.1	21.2	21.0	36.0	15.2	13.8
CCPS flashing SMD (µm)	97.2	197	119	119	264	97.9	90.6
CCPS mech. SMD (µm)	3.8	12.6	17.6	17.5	30.0	12.7	11.5
JIP proposed SMD (µm)	26.3	28.7	30.0	29.9	522	28.8	28.2

Table 1. Experimental conditions, measurements and model predictions for experiments

Figure 5 to Figure 11 include SMD graphs as function of superheat corresponding to the above experiments. The figures include the experimental data point and the results from the above type of correlations. In all the simulations the meta-stable liquid assumption has been assumed for the expansion from stagnation conditions to orifice conditions (meta-stable liquid), with flashing only occurring during the expansion from orifice to ambient conditions. Given the small L/D ratios, this assumption appears to be consistent with what was observed for most of the above experiments.

The following can be concluded from the table and the figures:

- 1) The TNO Yellow Book droplet size correlation results overall in significant over-prediction of the droplet size in conjunction with the conservation of momentum assumptions (as recommended in the new Yellow Book), while it results overall in significant under-prediction of the droplet size in conjunction with the isentropic assumption. If the meta-stable liquid assumption is not applied, different conclusions could be obtained.
- 2) In case the CCPS correlation is applied in conjunction with the meta-stable liquid assumption and conservation of momentum assumption, the droplet size is largely over-predicted. As a result, consistent with the UDM runs for the RELEASE book, the CCPS correlation should be applied with the meta-stable liquid assumption in conjunction with the isentropic assumption. Therefore the CCPS droplet size correlation is not recommended, since the isentropic assumption is not advised to be used (see Appendix A for details).
- 3) The CCPS book erroneously advises to take the minimum of the droplet sizes derived from the

ⁱⁱ Input data including (?) are presumed values not found from the literature; STEP involved saturated-liquid release

mechanical break-up and the flashing break-up correlations. This assumption results in too low prediction of droplet sizes, and therefore under-prediction of CCPS rainout (see Section 5). For the current validation it also results in incorrect behaviour for increasing superheat. As can be seen from the figures, in the sub-cooled region the minimum SMD is frequently predicted by the flashing correlation while in the superheated region it is frequently predicted by the mechanical break-up correlation. The above demonstrates the need for an appropriate transition criterion as proposed in the new JIP correlation.

- 4) For the Cardiff experiments the new JIP correlation provides naturally the most accurate results, since the correlation was fitted to these experiments. For the STEP experiment also close agreement is obtained, while the CCPS flashing correlation over-predicts. For the VKI experiment, the JIP correlation under-predicts less than the CCPS flashing correlation over-predicts. The JIP correlation more severely over-predicts the butane experiments than the CCPS flashing correlation. For Bigot's water experiments the CCPS flashing correlation slightly over-predicts, while the JIP correlation under-predicts.
- 5) It seems to be the case that for the low stagnation pressure (low velocity) of the BU-OR experiment the JIP correlation over-predicts, while for the higher pressures of other experiments it under-predicts. The CCPS flashing correlation has a general trend for over-prediction.
- 6) The accuracy of the new correlation could potentially be improved by modifying the form of the correlation between transition points. This would require significantly more droplet size measurements at various conditions of superheat.

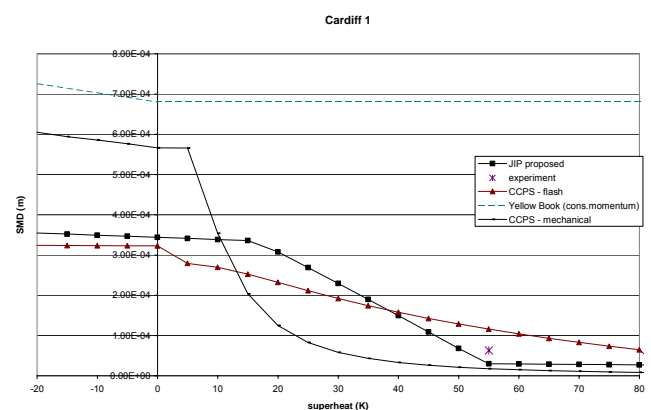


Figure 5. Validation of ATEX SMD correlations against Cardiff 1 experiment

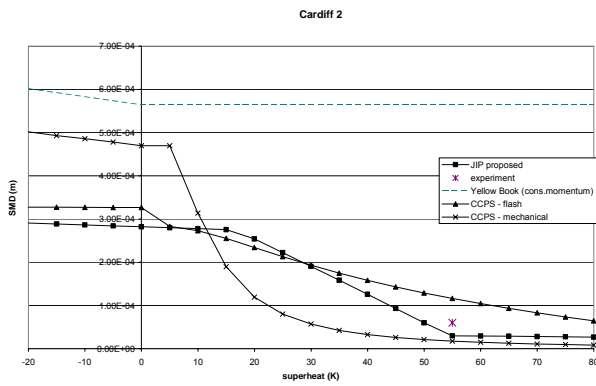


Figure 6. Validation of ATEX SMD correlations against Cardiff 2 experiment

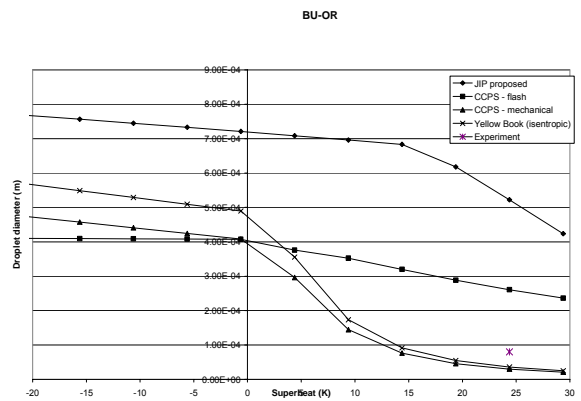


Figure 9. Validation of ATEX SMD correlations against BU-OR experiment

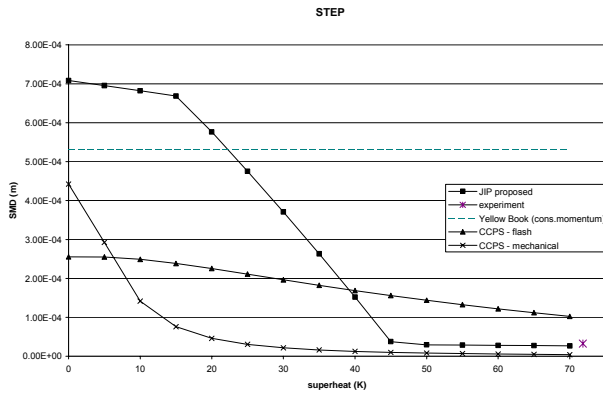


Figure 7. Validation of ATEX SMD correlations against STEP experiment

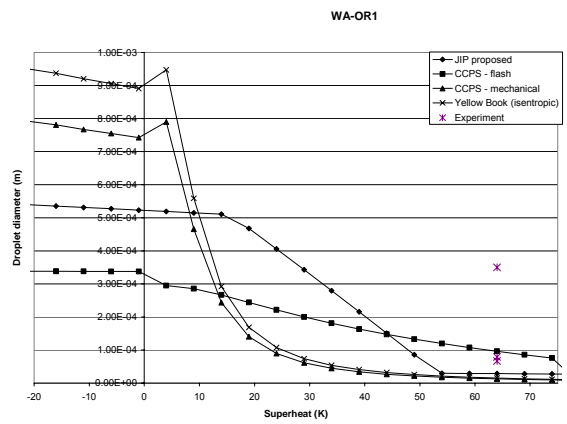


Figure 10. Validation of ATEX SMD correlations against WA-OR1 experiment

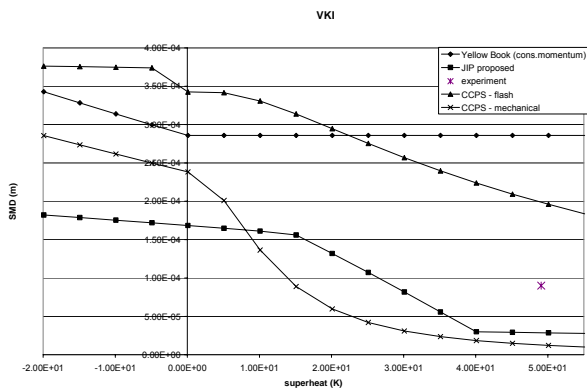


Figure 8. Validation of ATEX SMD correlations against VKI experiment

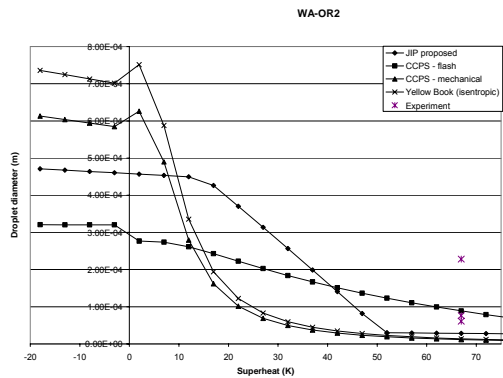


Figure 11. Validation of ATEX SMD correlations against WA-OR2 experiment

5. Modelling and validation of rainout

The PHAST two-phase dispersion model UDM^{2,3} obtains as input the ATEX post-expansion data (diameter, velocity, droplet size, etc.). The solution of the droplet equations in the UDM has been made more robust enabling an accurate solution of the droplet equations. This new UDM version will be made available in a version of PHAST in the near future.

This section summarises the validation of the UDM against the CCPS rainout data using both the original CCPS correlations as well as the newly proposed correlation. See the CCPS book⁹ for full details on the CCPS and MMA Rohm and Haas rainout experiments. In these experiments the orifice is reported as relatively sharp-edged, and the pipe preceding the orifice short and wide-bore to help suppress flashing. Thus $L/d_o=0$ can be assumed and the meta-stable liquid assumption can be applied upstream of the orifice. Ten of the experiments reported in the CCPS book were simulated in detail, i.e. 2 randomly chosen experiments for each of the 5 chemicals (flashing jets of water, CFC-11, chlorine, cyclohexane, monomethylamine).

First the droplet size was determined based on the experimental conditions reported in Appendix A in the the CCPS book⁹, whereby the orifice pre-expansion velocity is set from the measured flow rate. The results of this are presented in Table 2 in order of increasing superheat for both the CCPS flashing criterion and the newly proposed criterion. The SMD values for the CCPS flashing criterion are mostly in agreement with the CCPS book, but there are discrepancies for CFC and water.

	CFC11 - 8	Cyclohexane - 41	Chlorine - 22	Methylamine - 40	Chlorine - 20	Methylamine - 34	CFC11 - 5	Cyclohexane - 56	Water - 5	Water - 10
Superheat (K)	2	10	11	19	20	30	35	42	72	82
CCPS flashing	532	386	424	266	345	205	291	207	81	62
CCPS mechanical	1933	232	508	23	184	27	53	20	11	9
CCPS	532	232	424	23	184	27	53	20	11	9
Proposed JIP	1192	770	1008	84	677	184	272	30	27	26

Droplet size in μm



Table 2. Droplet size predictions for selected set of CCPS experiments

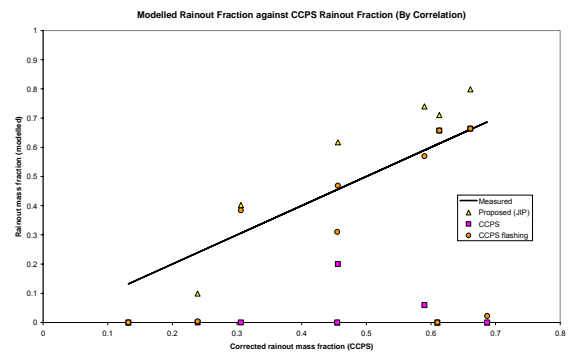


Figure 12. Modelled versus CCPS corrected rainout for the CCPS and the proposed correlations

Secondly the UDM was run based on the input data reported in Appendix A of the CCPS book⁹ and adopting the droplet size as calculated by ATEX (see above). The results of the predicted versus the observed rainout fraction are presented in Figure 12.

- It is seen that the CCPS flashing criterion agrees well with the experiments, which is understandable since it was fitted against these data. This is except for the water experiments, where the observed rainout was larger because of additional rainout of water from the humid air.
- Where the recommended CCPS criterion is adopted (taking the minimum of droplet sizes from mechanical and flashing break-up), a considerable under-prediction of rainout is observed.
- The accuracy of the new correlation is good considering it was not fitted against the data. In reality post-discharge liquid mass will be distributed through a range of droplet diameters. Smaller ones will evaporate rapidly, and larger ones persist and rain out. In the UDM, however, we assume droplets have a uniform initial droplet diameter, and all therefore evaporate at a uniform rate. Consequently rainout is likely to be oversensitive to droplet size, underestimating rainout for small droplets and overestimating rainout for large ones. This can be observed in Figure 12.

6. Future work

Phase II was limited to scaled experiments for water only with the emphasis on post-expansion measurement of the droplet size and derivation of post-expansion droplet correlations. Hence, the new correlation proposed is immature, and requires considerable further verification and development:

- A. Additional scaled experiments to ensure that the derived droplet size correlations are also valid for other chemicals than water – the influence of fluid properties have not been studied within the experimental programme. This would ideally include accurate characterisation of discharge and atmospheric expansion zone, and added downstream measurements such as droplet distribution, liquid fraction, concentration and rainout. It should also include a benchmark study for mixtures.
 - B. Large-scale experiments (for chemicals such as propane or butane). For real-life scenarios, these would give more confidence concerning predictions for droplet size, concentrations and rainout.
 - C. Model improvements. This should include added validation from the above scaled and large-scale experiments and likely further refinement of droplet size correlations. It would also include the appropriate application of equations for expansion from stagnation to orifice conditions [e.g. usage of non-equilibrium (meta-stable liquid) versus equilibrium], and expansion from orifice to ambient conditions [e.g. usage of isentropic versus conservation of momentum].
4. The above demonstrates the need for an appropriate transition criterion as is applied in the newly proposed JIP correlation. It was shown that overall the new correlation provided the most accurate results. It seems to be the case that for low stagnation pressures (low velocities) the JIP correlation over-predicts while for higher pressures it under-predicts. The accuracy of the new correlation could be further improved by improvements in the assumed form of the correlation between the transition points.
 5. The CCPS flashing droplet size correlation results in accurate predictions for the CCPS rainout experiments since it was fitted against the data. The result for the newly proposed correlation is good considering it was not fitted against the data.
 6. A further study has been proposed to consolidate and improve the modelling approach for flashing releases, which will provide confidence in predictions for (i) other materials (ii) larger scale/full scale.

Appendix. A. Modelling of expansion from orifice to ambient conditions

The expansion model calculates the final conditions at the end of the expansion from the initial conditions (see Figure 13). This problem has been reviewed and analysed by Britter^{23,24} and Van den Akker²⁵.

Within the control volume associated with the depressurisation zone for the one-dimensional, homogeneous flow (though not necessarily single-phase) in thermal equilibrium, the conservation of mass, momentum and energy lead to the following equations:

$$m_f = m_o \quad (13)$$

$$m_f u_f = m_o u_o + (P_o - P_f) A_o \quad (14)$$

$$m_f \left[h_f + \frac{1}{2} u_f^2 \right] = m_o \left[h_o + \frac{1}{2} u_o^2 \right] \quad (15)$$

where m_o , u_o , h_o , P_o , A_o and m_f , u_f , h_f , P_f , A_f are the flow rate (kg/s), specific enthalpy (J/kg), speed (m/s), pressure (Pa), area (m²) prior and after the expansion respectively; P_f is the pressure at the end of the flash region, and is therefore, equal to the ambient pressure P_a . P_o is the pressure at the exit plane of the orifice, which for flashing two-phase releases, is usually considered to be the saturated vapour pressure at the reservoir temperature.

7. Conclusions

1. A new empirical sub-model for predicting droplet size and size distributions from flashing jet releases has been proposed. The new droplet size correlation encompasses the regimes of mechanical break-up, transition between non-flashing and flashing, and fully-flashing jets. The new correlation is expressed in terms of orifice data, while the recommended correlations by CCPS and the Yellow Book are expressed in terms of post-expansion data.
2. In the regime of mechanical break-up, the new droplet-size correlation typically results in lower predictions than the CCPS and Yellow Book Weber-number correlations but larger values than those predicted by the Tilton and Farley and Elkoth correlations.
3. The CCPS book erroneously advises to take the minimum of the droplet sizes derived from the mechanical break-up and the flashing break-up correlations. In the flashing regime, this may result in significant under-prediction of the droplet sizes, while the CCPS flashing correlation has a general trend for over-prediction. The Yellow Book correlation significantly over-predicts in the flashing regime.

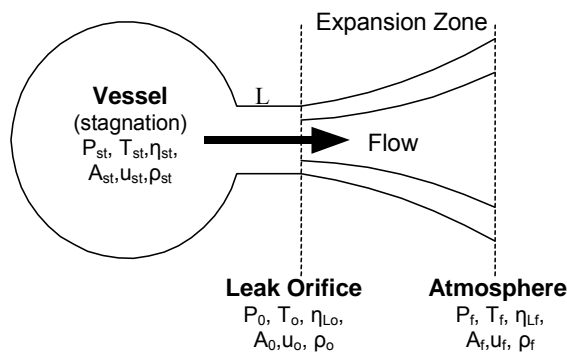


Figure 13. Control volume for atmospheric expansion to ambient pressure

Thus far, subject to the initial reduction of the problem (1-dimensional, homogeneous flow and thermal equilibrium), no further approximations have been introduced, and the system (13), (14), (15) may be referred to as the exact equations. These equations correspond to those included in HGSYSTEM and PHAST, and also corresponds to the formulation recommended by Britter^{23,24} and the TNO Yellow Book¹².

The ‘isentropic’ formulation recommended by Woodward in Perry’s Handbook²⁶ replaces the momentum equation (14) with the isentropic assumption, and is applied in conjunction with the meta-stable liquid assumption for the expansion from stagnation to orifice conditions. Thus it applies conservation of mass/entropy/energy during atmospheric expansion and no flashing occurs prior to the orifice with $P_o = P_a$, $T_o = T_{st}$. The CCPS droplet size correlation is based on this ‘isentropic’ assumption and therefore this correlation must always be used in conjunction with the isentropic assumption.

The advantage of using the so-called isenthalpic or isentropic assumptions is not clearly apparent, as there is little additional computational effort required to provide the exact solution for the control-volume approach. Hence, it is recommended that for present, in the case of flashing releases, the assumption of a pure liquid release at the exit orifice, together with the exact system [equations (13), (14), and (15)] be continued. Therefore usage of the CCPS droplet size correlation (which is derived using the isentropic assumption, i.e. not based on the exact system) is not recommended.

The main current weakness of the approach is considered to be the assumption of a single-phase liquid jet at the exit orifice. As discussed in other sections of this report, this is clearly not the case for many flashing releases, where nucleation and bubble-growth has already taken place upstream of the exit orifice. Hence, an additional methodology to determine the two-phase characteristics at

the exit orifice as outlined earlier, would provide the additional benefit of an improved model for the post-flash vapour mass fraction. An initial simple methodology has been recommended for this as part of the development of the newly proposed droplet-size correlation in this paper.

The other assumptions adopted in the overall 1-dimensional, homogenous, non-entraining approach could be appraised either experimentally by developing and utilising an appropriate LIF system, or numerically by comparing with CFD models. However, it is not immediately obvious how errors in the modelling philosophy identified through these studies could be used to improve the model. They would simply provide input to error analysis.

Nomenclature

A	cross-section area, m ²
C _p	specific heat, J/kg/K
d _d	Sauter Mean Diameter (SMD) = d ₃₂ , m
d _{da}	SMD based on aerodynamic (mechanical) break-up criterion, m
d _{df}	SMD based on flashing break-up criterion, m
d _o	orifice diameter, m
h	specific enthalpy, J/kg
h _{fg}	latent heat of evaporation (J/kg)
Ja	Jacob number, -
L	wall thickness (release from hole in vessel) or pipe length (pipe release), m
m	discharge flow rate, kg/s
P	pressure, N/m ²
P _v ^{sat} (T)	saturated pressure of released component at temperature T, N/m ²
Re	Reynolds number, -
T	temperature, K
u	velocity, m/s
We	Weber number, -

Greek letters

ΔT _{sh}	superheat, K
η	mass fraction, -
ρ	density, kg/m ³
σ	surface tension, N/m
φ	correction function to Jacob number in criterion for transition to flashing, -

Subscripts

a	ambient (atmospheric)
f	final (after atmospheric expansion)
L	liquid
o	orifice (immediately downstream of orifice, prior to atmospheric expansion)
sat	saturated conditions
st	stagnation (before expansion from storage data to orifice data)
v	vapour

Acknowledgements

Financial support of the work reported in this paper (Phase II project) was provided by DNV Software, Atofina, Gaz de France and RIVM. The contents of this paper including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect the policy of these organisations.

References

- ¹ Witlox, H.W.M. and Bowen, P.J., "Flashing liquid jets and two-phase dispersion - A review" Work carried out by DNV for HSE, Exxon-Mobil and ICI Eutech, HSE Books, Contract research report 403/2001 (2002)
- ² Witlox, H.W.M., and Holt, A., "A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation", International Conference and Workshop on Modelling the Consequences of Accidental Releases of Hazardous Materials, CCPS, San Francisco, California, September 28 – October 1, pp. 315-344 (1999)
- ³ Witlox, H.W.M., and Holt, A., "Unified Dispersion Model", Technical Reference Manual, Version 6.0, DNV, London (2000)
- ⁴ Muralidhar, R., Jersey, G.R., and Krambeck, F.J., "A Two-Phase Model for Subcooled and Superheated Liquid Jets", International Conference and workshop on modelling and mitigating the accidental releases of hazardous materials, AIChE, CCPS, New Orleans, LA, September 26-29, pp. 189-224 (1995)
- ⁵ Muralidhar, R., Jersey, G.R., and Krambeck, F.J., "A two-phase release model for quantifying risk reduction for modified HF alkylation catalysts", *J. of Haz. Mat.* **44**, pp. 141-183 (1995)
- ⁶ Witlox, H.W.M., Bowen, P.J., Cleary, V.M., and Harper, M., "Two-phase release and atmospheric dispersion – Phase II", Contract 41008300 for RIVM (Dutch Government), Gaz de France and Atofina, DNV, London (2004)
- ⁷ Witlox, H.W.M., Bowen, P.J., Cleary, V.M., and Harper, M., "Flashing liquid jets and two-phase droplet dispersion", Paper 4 in proceedings of "Major Hazards Offshore and Onshore", December, London (2004)
- ⁸ Ramsdale S.A. 'Droplet Formation and Rainout from Two-phase Flashing Jets', AEAT-2124 Issue 1 (1998)
- ⁹ Johnson, D.W., and Woodward, J.L., "A model with data to predict aerosol rainout in accidental releases", Center of Chemical Process Safety (CCPS), New York (1999)
- ¹⁰ Brown, R. and York, J.L., "Sprays formed by flashing liquid jet", *AIChE J.*, **8**, pp.149 –153 (1962)
- ¹¹ Heinze, J.U., "Fundamental of the hydrodynamics mechanisms of splitting in dispersion processes", *AIChE J.*, **1**, pp. 289-295 (1955)
- ¹² van den Bosch, C.J.H., and Duijm, N.J., Sections 2.3.4.6, 2.4.3.5, 2.5.3.7 on 'Finite-duration spray releases' in "Outflow and Spray Release", Chapter 2 in "Methods for the calculation of physical effects - TNO Yellow Book", CPR14E, Third Edition, Committee for the Prevention of Disasters, SDU, The Hague (1997)
- ¹³ Appleton, P.R., "A study of axi-symmetric two-phase flashing jets", report R303, SRD, Culcheth, Warrington, Cheshire, UK (1984)
- ¹⁴ Wheatley, C.J., "Discharge of liquid ammonia to moist atmospheres – survey of experimental data and model for estimating initial conditions for dispersion calculations", report R410, SRD, Culcheth, Warrington, Cheshire, UK (1987)
- ¹⁵ Kitamura Y., Morimitsu H., and Takahashi, T., "Critical Superheat for Flashing of Superheated Liquid Jets", *Ind. Eng. Chem. Fundam.*, Vol.25, No. 2. pp. 206-211. (1986)
- ¹⁶ Tilton J.N., and Farley C.W., "Predicting Liquid Jet Break-Up and Aerosol Formation During the Accidental Release of Pressurised Hydrogen Fluoride", *Plant/Operations Progress* 9-12, p.120 (1990)
- ¹⁷ Elkotb M.M., "Fuel Atomisation for Spray Modelling", *Prog. Energy Combust. Sci.* **8**-1, pp. 61-91 (1982)
- ¹⁸ Hervieu, E. and Veneau, T., "Experimental determination of the droplet size and velocity distributions at the exit of the bottom discharge pipe of a liquefied propane storage tank during a sudden blowdown", *J. Loss Prev. Ind.*, Vol. 9, No. 6, pp. 413-455 (1996)
- ¹⁹ Vandroux-Koenig, S., and Berthoud, G., "Modelling of a two-phase momentum jet close to the breach, in the containment vessel of a liquefied gas", *J. Loss Prev. Ind.*, Vol. 10, No. 1, pp. 17-29 (1997)
- ²⁰ Yildiz D, Rambaud P., van Beeck J. 'Break-up, Droplet Size and Velocity Characterisations of a Two-Phase Flashing R134A Jet', 5th International Conference on Multiphase Flow (ICMF'04), Yokohama, Japan, May 30-June 4, Paper No. 408 (2004)
- ²¹ Touil, A., Bigot, J.P., Bonnet, P., Lacombe, J.M., and Duplantier, S., "Rainout prediction: initial droplet diameter experimental determination", pp. 3201-3309, *Loss Prevention and Safety Promotion in the Process Industries*, 11th Int. Symp., Prague, 31 May – 3 June 2004 (2004)
- ²² Bigot, J.P., "Private communication", June 2005 (2005)
- ²³ Britter, R.E., "Dispersion of two-phase flashing releases - FLADIS field experiments; a further note on modelling flashing releases", Report FM89/3 by CERC for EEC Commission DGXII (1995)
- ²⁴ Britter, R.E., 'Dispersion of two-phase flashing releases - FLADIS field experiments; the modelling of pseudo-source for complex releases', Report FM89/2 by CERC for EEC Commission DGXII (1994)
- ²⁵ Van den Akker, H.E.A., Snoey, H., and Spoelstra, H., "Discharges of pressurised liquefied gases through apertures and pipes", *IchemE Symposium Series* **80**, pp. E23-E31 (1983)
- ²⁶ Perry, R.H, Green, D.W. and Maloney, J.D., (eds.), "Perry Chemicals Engineering Handbook", 7th Edition, McGrawhill (1999), Section 26 "Process safety"