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Flashing liquid jets and two-phase dispersion

A review

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The aim of this review is to determine whether current approaches and practice for modelling accidental atmospheric 'flashing' jet releases and subsequent dispersion - including possible rain-out - is consistent and up-to-date with information in the public domain. The study focuses on the two-phase aspects, with emphasis on flash atomisation and droplet dynamics downstream. Industrial processes and problems where similar thermo-fluid processes prevail are included within the remit. One essential outcome of the work is a proposal for an optimised and prudent strategy to develop quantitative methodologies for these problems in the short, medium and longer term. Several high-profile studies have been undertaken in this area over the last decade, so clear statements are required to explain where and why deficiencies still remain.

The review considers models and validation data for the sub-processes of atomisation, atmospheric expansion to ambient pressure, two-phase dispersion, rainout, pool formation and re-evaporation. Most significantly, the source term for the downstream dispersion calculations are currently ill-defined due to lack of a justifiable, validated atomisation model, and no large-scale data-set for releases with significant rainout exists which links the initial post-expansion conditions with downstream rainout or airborne concentration. Only two models have been found which attempt to model the primary two-phase processes on a physical basis, the DNV 'Unified Dispersion Model' and its multi-compound generalisation by Exxon-Mobil; potential limitations of these models are discussed. Several correlations have been proposed which predict final rainout directly from initial release conditions, and these may be useful for engineering guidelines in the short term.

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1. INTRODUCTION

This report has been commissioned by Det Norske Veritas Ltd. with financial support from the UK HSE, Exxon-Mobil (USA), and ICI Eutech (UK). The aim of the programme is to ascertain whether current two-phase modelling practice and philosophy adopted for the problem of accidental atmospheric dispersion releases of 'flashing' substances, as utilised in the dispersion code UDM, is consistent and up-to-date with literature in the public domain. Not only atmospheric dispersion literature is considered, but also developments from other industrial processes and problems where similar or identical thermo-fluid processes prevail. Furthermore, in light of the current state-of-the-art, the report aims to propose an optimised and prudent strategy for future development of quantified tools and techniques in this area in the future.

Several recent studies have been undertaken in this area, most notably :

- a multi-industry American initiative involving experimentation and analysis co-ordinated by the Centre for Chemical Process Safety (1989-1999)
- an EU contribution via the so-called STEP programme (1993-1997)
- a programme undertaken by the UK Health and Safety Laboratory (1995-2000)
- two reviews sponsored by the UK HSE undertaken by the UK Atomic Energy Authority (1998-2000)

Clearly with so much effort already having been expended in progressing towards understanding these complex problems, particular attention has to be paid to these specific studies, and clear statements are required to explain where and why deficiencies still remain.

1.1 BACKGROUND

PHAST: flash calculations and subsequent UDM droplet modelling

The latest Version 6.0 of the DNV Consequence Modelling Package PHAST was released early 2000. It includes models for discharge of hazardous chemicals to the atmosphere. For pressurised liquid releases from vessels and/or pipes, the final part of the PHAST discharge model is the 'flash model' which calculates the depressurisation (external expansion; flashing) from the exit pressure to the ambient pressure; see Figure 1a. The flash model outputs the post-flash data (liquid fraction, temperature, velocity, droplet size). Note that in addition to 'liquid-two-phase' expansion, the PHAST external expansion model also deals with other types of expansion (e.g. gas-gas expansion).

In PHAST6.0, the Unified Dispersion Model (UDM) calculates the subsequent dispersion of the two-phase cloud; see Figure 1b. It includes a unified model for jet, heavy and passive two-phase dispersion including possible droplet rainout, pool spreading and re-evaporation. It calculates the phase distribution and cloud temperature using either a non-equilibrium thermodynamics model, a non-reactive equilibrium model, or an equilibrium model specific for HF (including effects of polymerisation). Except for HF, it does not currently allow for reactions. Multi-compound mixtures can currently only be modelled very simplistically assuming a 'pseudo-compound' with 'averaged' properties.

Recent review of PHAST two-phase droplet modelling; literature review

Following a recent detailed assessment, revision and improvement of the UDM[1,2], further possible improvements (after PHAST6.0) were identified for the pre-UDM flashing calculations, the droplet modelling, rainout, pool spreading/evaporation, and the link between pool and dispersion model:

- The PHAST6.0 external expansion model is based on a set of assumptions and equations for the expansion zone (e.g. no air entrainment; conservation of mass, momentum and energy, etc.). There is some uncertainty in the literature regarding the precise assumptions to be adopted for the flashing (expansion) calculations.

  - The assumption of isentropic expansion versus isenthalpic expansion; see e.g. Van den Akker et al.[3], Britter[4], and the TNO yellow book[5].

  - The PHAST6.0 initial droplet size correlation assumes two possible mechanisms for droplet formation, i.e. "mechanical or aerodynamic" break up (droplet diameter given as function of the critical Weber number) and "flashing" break up (droplet diameter given as a function of the partial expansion energy). The model selects the droplet diameter calculated by the mechanism that gives the smallest value. The flashing break-up correlation is based on the CCPS rainout experiments[6,7]. Several shortcomings of this formulation have been identified in Section 4.1 in the UDM Thermodynamics Verification Manual (Section IIB of the UDM Technical Reference Manual[2]). These shortcomings were further confirmed by an external review by Webber[8]. See also the review of the RELEASE model and the CCPS data by HSE/AEA.[9] Alternative formulations are given by the TNO yellow book[5], Wheatley[10], and Appleton[11].

  - The entrainment of air from a sub-cooled non-flashing, liquid release through an orifice as well as air entrainment from the liquid mist droplets themselves can effect rainout by reducing the size of large droplets (see papers by Ricou & Spalding[12] and St.George & Buchlin[16]). It is also important to quantify the additional air entrainment and to investigate the effect of orifice characteristics.

- The current UDM assumes a single averaged-size droplet diameter, with 100% rainout of all liquid if the droplet hits the ground. Typically there would be a droplet distribution (mean and variance)[13], not all droplets would rain out at the same downwind location, and only droplets with a larger diameter would rain out.

- The UDM does currently only allow modelling of dispersion from an evaporating pool following rainout. This does not allow modelling of dispersion directly from a pool. Dispersion from a pool can be modelled indirectly by assuming a liquid release at ground level (resulting in immediate 100% rainout).

- Following re-evaporation from the pool, the UDM may assume a certain initial dilution. Overall it is considered that the link between the pool and the dispersion model needs further investigation and development.

Note in this context also should be mentioned the droplet measurements and associated modelling carried out as part of the EEC project STEP[14,15] (flashing propane jets), by the Von Karman Institute[16] (water sprays), and by Mobil[17,18] (flashing jets for multi-compound mixtures of HF and additive)

Current work

As a result of the current status outlined above it is believed that there are weaknesses in the approach adopted by contemporary dispersion codes in the manner in which the liquid-phase component is modelled. In particular, the near-source atomisation processes are considered ill-defined, and liquid rainout fraction near the source is a parameter of specific interest as this influences the quantity of hazardous material which remains an airborne hazard as the plume disperses. However, it is not clear whether, in light of general atomisation and spray technology, any improved methodology could be proposed with any greater satisfaction. Thus the essential remit of this report is to determine whether the modelling of liquid component processes within flashing two-phase releases could be

(a) improved immediately in light of methodologies or models currently available within the literature and
(b) recommend strategies to develop towards improved models of these processes in both the medium and long term.

1.2 SCOPE OF WORK PROGRAMME

The scope of work defined in this report represents Phase I of a Joint Industry Proposal. The deliverable of Phase I has been planned to lead directly into a kick-off meeting for potential further phases of work. The objective of this specific work programme is to establish state-of-the-art and provide recommendations for:

- external expansion model (particularly for initial droplet size, isentropic versus isenthalpic expansions; post-flash data are initial droplet size, flash fraction, velocity)
- air entrainment from jet releases and from liquid droplets
- droplet equations (including droplet distribution)
- rainout criteria (including cut-off diameter)
- pool formation and re-evaporation from pool
- other practical influences, e.g. orifice characteristics

This work will include a detailed literature review, including all references mentioned in Section 1.1. This will include the current UDM logic, as described in Chapter 4 in the UDM Thermodynamics Theory Manual and Chapter 4 in the UDM Thermodynamics Verification Manual (Sections IIA and IIB of the UDM Technical Reference Manual[2]). Further it will advise on best practice for modelling air entrainment from flashing jets based on current understanding. It will identify strengths/weaknesses of current models, and identify possible alternative modelling approaches. Finally it will provide clear recommendations.

This report has been designed to provide a logical progression through the basic physics of the problem, whilst remaining consistent with the objectives specified above. In Chapter 2, an introduction to the problem and description of the underlying thermophysics is provided. As many of the studies reviewed rely heavily on advanced laser diagnostic techniques, a brief review of appropriate diagnostic methodologies with reference to particular strengths and weaknesses of each is provided in chapter 3. This chapter is then used as a reference throughout the remainder of the report, and also serves to provide a basis for recommendations for future development. Chapters 4 and 5 represent the main body of the review for the near-source processes of atomisation and flashing, and chapter 6 and 7 similarly provide the technical discussion in relation to downstream droplet processes, rainout and re-evaporation. Chapter 8 presents the deliverables of the work programme in providing conclusions and clear recommendations of what represents the current state-of-the-art, and prioritisation of

outstanding weaknesses with, where evident, recommendations of how to address these systematically and prudently.

2. PHYSICAL PHENOMENOLOGY

2.1 DISCHARGE SCENARIOS

The practical problems considered under the remit of this programme are shown schematically in Figure 1. A breach of containment is considered, which results in depressurisation of the effluent through a final orifice of diameter up to 0.1m. The flow conditions at the orifice may be choked or un-choked depending upon initial conditions. Only steady conditions are considered within this report, though it is envisaged that the findings from this steady flow study will provide insight regarding likely consequences in the transient or instantaneous cases.

As an example, a typical scenario would be depressurisation of a large containment of Liquefied Propane Gas (LPG) to ambient atmosphere from a pressure of 6 bar through an orifice of 0.01m.

2.2 THERMODYNAMIC BOUNDARY CONDITIONS

The scenario under consideration comprises a pressurised containment of a liquefied substance of any thermodynamic state. This problem may be represented in various ways schematically. Here, the elementary input variables likely to be available to users of dispersion models are taken to generate the series of schematics shown in Figure 2.

The saturated conditions for a particular substance are superimposed on this schematic, whereupon crossing the effective 'transition' curve results in a change of phase. Hence, for all scenarios considered within the scope of this report, the pressurised 'contained' conditions (conditions 1) upstream of the release point (i.e. the stagnation conditions) lie above the liquid/vapour phase-change line, but to the right of the solid/liquid phase-change line. The initial and final conditions of any problem considered within the scope of work may be represented on this or similar phase-change diagrams, depending upon the chosen control variables. Condition 2 represents the final or far-field atmospheric condition into which the release disperses. The value of the so-called degree of superheat (ΔT_{sh}) of a contained liquid may now be evaluated by drawing a horizontal line from condition 2 on the schematic, until the liquid-vapour phase transition curve is met (i.e. at $T_{sat}(P_a)$). If the temperature at this intersection point is less than the initial stagnation temperature of the liquid, then the release is defined to be superheated, with the degree of superheat equal to $\Delta T_{sh} = T_{st} - T_{sat}(P_a)$. If the liquid is released into standard atmospheric conditions, then this simply represents the amount the stagnation temperature exceeds the normal boiling point of that liquid ($\Delta T_{sh} = T_{st} - T_b$).

Though a fairly elementary representation, this allows processes occurring during depressurisation across the nozzle and exit orifice now to be represented. The initial state of the liquid is termed 'sub-cooled'. Pressure decreases as the liquid approaches the exit, and if the fluid conditions remain above the liquid/vapour transition line, then in most cases (cavitation being the exception) the liquid remains subcooled, atomising as a single-phase homogeneous jet which disintegrates through aerodynamic interaction and wave instabilities at the liquid surface. Heat and mass transfer are subsequently controlled by droplet surface evaporation, forced convection and radiation processes downstream. The various mechanisms associated with jet break-up under these conditions are collectively termed 'mechanical' jet break-up. This type of jet break-up has received considerable attention in the literature, mainly for high pressure and small orifice (>100 bar; < 0.3mm) conditions of relevance to the automotive industry for direct injection engines, though a recent report[19] has extended the range of applicability.

A more complex scenario may now be envisaged if one considers again initial conditions above the liquid/vapour phase change line, but with final downstream conditions below the phase line – Figure 2b. If $\Delta T_{sh} > 0$, thermodynamic conditions within the nozzle at some point reach 'superheated' conditions, where the pressure has dropped below the local saturated vapour pressure. Under suitable conditions, the so-called 'flashing' process now commences, although as will be seen subsequently, often there is a delay in vapour production within the jet until a transitional superheat condition has been exceeded. If the fluid is actually stored under saturated conditions as a two-phase mixture, then the situation represented by Figure 2c is realised, whereby the fluid is stored under saturated conditions and released as a two-phase mixture.

Experimentalists wishing to investigate 'flashing' contaminants, which under standard atmospheric conditions exist as vapours, often utilise water as the model fluid, not least for safety reasons. This may initially seem unjustified, but through reference to Figure 2, some explanation may now be offered in terms of the similarities between releases of superheated water and liquefied vapours. Both may be stored at pressures elevated pressures under conditions that ensure their respective initial states are above the liquid/vapour transition curve. Essentially, as the initial upstream stagnation pressure is increased, then it may be observed that temperatures may be chosen for either fluid that will ensure the flashing conditions are encountered upon release into the open atmosphere i.e. such that ΔT_{sh} is positive. Of course the quasi-experimental equivalence is only likely to hold for the flashing process itself, the fluid's atmospheric state becoming more significant further away from the orifice during the post-expansion region. Note that for water this means that both initial and final states are above the liquid/vapour transition curve.

Finally, it is noted from Figure 2 that another way of achieving superheated 'flashing' conditions for an event which would otherwise remain sub-cooled when released into standard atmospheric conditions, is to reduce the ambient pressure, and hence lower the final exit conditions until ΔT_{sh} becomes positive. Experimentalists often utilise evacuated containers to invoke superheated conditions using this methodology, which would not be achievable under standard atmospheric conditions.

2.3 MICRO-PHENOMENOLOGY DURING FLASH ATOMISATION

Flash atomisation – as opposed to flashing (or superheated) conditions – may be visualised in the photographs provided by Reitz[20] in Figure 3. It is initiated at the so-called 'inception' stage of flashing, by the creation of very small bubbles - nucleation. Under release conditions of low superheat, nucleation is believed to occur outside the release exit – the so-called 'external' mode. At higher superheat conditions the bubble inception process occurs within the nozzle, via one of two inception mechanisms : (1) homogeneous nucleation via molecular processes throughout the body of the fluid, or (2) heterogeneous nucleation based on liquid/solid surface interaction on the walls of the orifice. As the bubbles flow towards the nozzle exit, they grow at a characteristic bubble growth rate. Depending upon the initial thermodynamic conditions (degree of superheat), and orifice geometric characteristics (particularly the length-to-diameter ratio of the discharge pipe), these initial droplets will have different fates. The fate of bubbles from internal nucleation may be represented as shown by the schematic in Figure 4 from Parks and Lee[21], which essentially summarises the findings of a systematic photographic study showing the dependence of internal flow structure on external spray formation.

At low superheat conditions – but still high enough to induce 'internal' nucleation – bubbles are observed to form near the nozzle's surface. When ejected through the end orifice, these bubbles shatter near the edge of the jet, but there still remains a significant 'liquid core', a characteristic of the mechanical break-up phenomenon under low pressure releases. As the degree of

superheat is increased, then more and more bubbles are created, eventually pervading the whole liquid jet. At some point the bubbly flow so created becomes so dense that bubbles merge with each other to produce the so-called 'slug flow'. Increasing superheat still further leads to annular flow at the nozzle exit, where liquid flows along the wall with an air core in the centre. Each of these modes results in different mechanisms for atomisation downstream, as demonstrated in recent studies of similar processes occurring within effervescent atomisers[22].

Beyond the release exit, various modes of atomisation prevail depending upon the flow conditions upon release. Bubble-bursting, ligament formation with subsequent break-up, and liquid sheet break-up can all play roles depending upon flow regime. The atomisation process is typically considered to be complete within about 100 orifice diameters downstream, though correlations have been developed to estimate the break-up length more accurately.

Vapour production may be considered to occur concurrently with the atomisation process. This is usually modelled during the 'flash' phase as being a non-entrainment region - Figure 1a. In this region, conservation equations of mass, momentum and energy (or approximated to enthalpy or entropy) govern the relative phase contribution and velocity at the pseudo-source.

2.4 FATE OF DROPLETS AFTER ATOMISATION

Figure 1b represents the processes occurring during the subsequent dispersion of the two-phase jet. The jet expands downstream due to the turbulent entrainment of air, which may result in further vaporisation of droplets, and which in turn cools the jet to due to the effect of latent heat. The droplet population provide a two-way interaction between themselves and the gaseous environment exchanging heat and mass, and also due to their exit momentum and buoyancy follow differing trajectories which will determine whether they remain in suspension, or settle out (rain-out) in the near-field, possibly giving rise to a spreading and vaporising liquid pool.

2.5 ANALOGIES WITH OTHER TWO-PHASE INDUSTRIAL PROCESSES

Processes from several different applications have been considered due to perceived analogies with the current problem, and hence potential for utilising understanding and interpretation in these related areas to elucidate flashing jet atomisation in dispersion problems.

A similar sequence of processes has recently been identified in an atomisation method which utilises two-phase bubbly flow analogous to flashing jet releases, but with the gaseous phase introduced mechanically under isothermal conditions. Exactly the same processes are encountered as air-to-liquid mass ratio (or void fraction) in the mixture is systematically increased. Moreover, this results in step changes in atomisation trends as transition between different modes is realised[22]; tree-like ligaments have been observed to form under annular flow conditions, whereas for lower air-to-liquid ratios, bubble-bursting is the main mechanism identified beyond the exit orifice. There is a considerable body of data available for these types of atomisers with associated correlations for characterising atomisation as a function of upstream flow conditions. It seems plausible that once the two-phase flow has been established, atomisation may be controlled by the highly dynamic physical processes such as expansion and shattering of bubbles rather than further thermodynamic influence. If these analogies could be substantiated, then considerable time and cost savings could be accrued in developing a validated model of two-phase flashing jets. Figure 5 shows the flows observed just downstream of the exit orifice of an effervescent atomiser. Clearly parallels exist with the flow regimes encountered in flashing nozzles as superheat increases, effectively increasing the void fraction at the exit orifice.

Heat transfer processes for two-phase flows has received considerable attention, most prominently in relation to predicting performance of heat exchangers. Considerable work has been undertaken studying the thermodynamics of nucleation and bubble-generation within tubes, characterisation of the various two-phase flow regimes encountered, and other relevant processes such as pool boiling. For example, Hewitt[23] provides Figure 6 to characterise the flow transition under conditions of constant heat flux as the flow develops downstream. Analogies may be made with reference to Figure 2 where the first scenario could be envisaged to be a sub-cooled release. As the superheat (heat flux in this analogy) increases, then different flow conditions will be encountered, as anticipated for flashing jets. These flow regimes are also consistent with those reported for effervescent atomisation, so again it seems plausible that downstream atomisation processes corresponding to the various two-phase flow conditions identifiable in Figure 6 prevail.

Albeit on a considerably smaller scale, there are notable similarities between the two-phase dispersion problem and the two-phase fluid dynamics of fuel injection in automotive engine cylinders or gas turbines. Indeed, the majority of progress in understanding sprays, atomisation and transport of droplets has been driven by these applications[24,25]. Many of the references and developments reported in this review will have been derived with fuel injection being the primary application.

Cavitation is another two-phase process associated with atomisation, which may be considered as an analogous process to flashing. Cavitation is known to exist during pressurised injection of liquid into an ambient atmosphere, when local conditions within the exiting passage drop below the localised saturation pressure. This results in the creation of vapour bubbles. However, Dumont et al.[26] report that the bubbles created within the atomiser rapidly disappear in the dense liquid core of the atomising jet, and that the primary influence of cavitation in terms of its direct effect on atomisation is believed to be the increase in exit velocity through the cavitation-induced vena contracta. Hence, for the purposes of this report it is concluded that no benefit may be gained by analysing the cavitation process further.

Finally, a brief review of atomisation research concerning liquid propellants for application in the rocket propulsion industry was undertaken. As for the cavitation process, no information of direct use in developing flash atomisation understanding was identified, and so further analysis of progress in this area was aborted.

3. EXPERIMENTAL METHODS FOR FLASH INVESTIGATIONS

The majority of experimental results discussed in the following sections, and those proposed for future studies, rely upon laser-based techniques in order to derive trends, correlations of data or valid benchmark data. Hence, it is appropriate to briefly introduce the various relevant diagnostic techniques, so they can then simply be referenced throughout the remainder of the report during discussion.

Diagnostic techniques, in particular laser-based diagnostic techniques, for single and two-phase fluid dynamic problems have been introduced and rapidly developed over the last 25 years so that a healthy balance currently exists between modelling and empirical studies. A considerable advantage of laser-based techniques is their non-intrusive nature, their data-acquisition rates, and speed of processing. For example, now fuel injectors which deliver fuel typically over milli-second time periods, with droplet speeds exceeding 100 m/s, and containing droplets with sizes from 1-100μm can be characterised on a transient basis[27]. However, all laser-based techniques have inherent inaccuracies which need to be acknowledged and properly accounted for in appropriate experimental studies. Excellent thorough reviews of these techniques are provided in the treatise edited by Chigier[28].

3.1 TYPES OF MEASUREMENT TECHNIQUES

3.1.1 Droplet Sizing

Sample Collection and Post-Analysis

These were the only methods available to derive droplet size distributions before the introduction of laser techniques. They are still of use today in hostile environments where the use of laser-based techniques would not be possible or inappropriate. A typical example is the magnesium-oxide powdered slide, which is exposed to the two-phase flow for a short period of time before being mechanically covered again to protect the data. Droplets in the flow impinging on the plate leave imprints which are subsequently analysed manually (more recently with the aid of image analysis software) to produce spray statistics. Another variant is the method of freezing the droplets in a wax or similar (e.g. Silicon Oil used by Peters et al.[29]), ready for post-analysis. Where practicably possible, these methods have been and should continue to be superseded by laser diagnostic techniques.

Laser Diffraction-Based Techniques

The basic principle of the technique was first reported by Swithenbank et al.[30], and atomisation and spray research has relied on the commercial version (marketed primarily by Malvern Instruments, UK) ever since. The basic principle relies the fact that diffraction angles of incident mono-chromatic light vary according to droplet size - larger diffraction angles correspond to smaller droplets. Using Fraunhofer theory, this angular variation can be calibrated and quantified, and with the aid of a Fourier-Transform lens, the optical system allows a spatially integrated temporal measurement of spray distribution along a line-of-sight.

There are inherent inaccuracies associated with diffraction-based techniques which have to be accounted for in any experimental set-up. The so-called ‘vignetting’ effect occurs due to inappropriate selection of object-to-collection-lens distance in relation to droplet sizes present, whereby diffraction angles of the smallest droplets are such that they pass outside the diameter

of the collection lens. This effect can be minimised by selecting appropriate measuring distances, and for larger-scale applications, this often means shielding sections of the spray, with an obvious compromise in terms of obtrusiveness. Alternatively, a non-standard collection lens larger than standard may be applied[31] to ensure that droplets are measured from even the widest collection angles (smallest droplets). A second common source of error in diffraction-based measurements concerns the spray density. The so-called 'obscuration' encountered in diffraction measurements can induce gross errors for dense sprays. Calibration equations have been proposed to allow post-processing of measured data in dense sprays to obtain more accurate estimates[32].

Both inherent errors associated with the diffraction technique need to be considered before being applied to the investigation of flashing jets. As it is well-known that the cone-angle expands when flashing occurs – meaning that optical configurations will have to be positioned further away or within the spray itself – and that the initial spray is very dense, research presenting diffraction-based data from flashing jets should explain the influence of these two effects on data, and how they were accounted for in practice.

Imaging Techniques

Included in this category are high-magnification photography methods, holographic methods, Interferometric Laser Imaging for Droplet Sizing (ILIDS), etc.. Usually high-powered lasers (e.g. the 'Nd:YAG' laser family) are utilised due to the non-linear relationship between image intensity and droplet size. In this sense, the techniques should be biased towards larger particles, methods for accounting for out-of-focus droplets need to be resolved, and data-processing times are invariably longer than the quasi-real time generation of other techniques. Direct imaging can also be helpful in regions where non-spherical droplets pervade.

Phase Doppler Anemometry (PDA)

This basis of this technique was first reported by Bachalo[33]. Systems relying on the same basic principle but with optimised electronics and post-processors are now marketed by companies such as Aerometrics, Biral and DANTEC. The technique involves setting up an interferogram in space by overlapping two mono-chromatic, similarly polarised beams, which subsequently provide Doppler signals as droplets pass through them. Collecting signals from different receiving angles, the size of the droplets can be calculated from geometric analysis. Several errors would be encountered utilising this basic principle, so that in practice the interferogram is configured to move with a constant velocity. Moreover, signals are collected from several positions to eliminate the so-called phase ambiguity problem. Even with these safeguards, still further sources of error may be incurred, including non-spherical droplets (the technique is only directly appropriate for spherical droplets) and multiple occupancy in the measurement volume. A measurement dynamic range is typically of the order of 100, so that several experiments would have to be constructed if a very broad distribution of sizes was required. A significant advantage of the PDA technique is that when appropriately configured, up to 3 components of velocity can be measured as well as size distributions concurrently. Furthermore, the information is provided effectively at a point (in reality over a very small volume) in space, allowing spatial resolution. Temporal resolution can be afforded with additional post-processing of data for events with a natural or artificially-imposed frequency, such as automotive injectors[27] . Hence, data can be provided in the case of impulsively started jets, which are a particular category of hazard in risk assessment. There is a limitation in terms of spray density for which the technique is appropriate, so that it will not be viable for measurements to be taken very close to the orifice for flashing-jet releases.

Planar Droplet Sizing Techniques

Recent developments have considered the integration of Mie and Fluorescent (see LIF following) planar sheet diagnostics to arrive at an instantaneous 2-dimensional planar map of droplet size. This technique is under development and progress should be monitored for future application to the problem of flashing jets, though the spray density is likely to cause problems for this technique, as for the others already mentioned.

3.1.2 Mass Fraction and Relative Vapour Fraction

Differential Infra-Red Absorption (DIRA)

This technique is essentially a 'line-of-sight' technique first reported by Shell Research Ltd.[34] for measuring the preferential evaporation of lighter components in internal combustion engines. The basis of the technique is that a beam of near infra-red radiation is passed through a two-phase mixture, which will be absorbed by the vapour phase radiation according to the Beer-Lambert law, and scattered or absorbed by the droplets or optical components within the line-of-sight. The undesirable second component of attenuation may be extracted from measurements by splitting the beam and passing through optical filters to measure at a wavelength where absorption is negligible. As this wavelength, attenuation is due to effects other than molecular absorption, and so the vapour-phase concentration may be derived. This technique could be considered for development in the context of the current problem.

Laser-Induced Fluorescence (LIF)

This technique involves passing a high intensity laser-sheet through a single or two-phase mixture at a suitable wavelength and with sufficient energy to provide an energy release at a different wavelength, either from fluorescence of the fluid itself or more usually from a tracer dopant for the fluid. The choice of a suitable dopant is usually considered the critical aspect of the technique. A 2-dimensional image of fluorescence from a planar sheet of laser light is then recorded using suitable imaging hardware, which usually has to include hardware to intensify the signal due to the low fluorescent energies emitted. Image analysis software is then employed for calibration and to convert the image characteristics into the relevant quantifiable variable. One particular inherent problems include the variation of fluorescent energy as the radiation passes through the measurement region. This basic technique has been shown to be suitable to be extended to provide measurements of vapour fractions in 2-phase mixtures (EXCIPLEX) or mixture temperatures[35]. These are non-trivial extensions to the basic method, though should still be considered as techniques under development.

3.1.3 Velocity and Turbulence

Of the techniques already discussed, PDA and direct photography allow derivation of kinematic information in addition to droplet sizing. PDA explicitly constructs the optical configuration such that only components of velocity in orthogonal directions are measured (Laser Doppler Anemometry, LDA). Hot-wire technology is another well-developed though intrusive technique, and for which problems may be encountered in two-phase thermodynamically unstable flows.

Particle Imaging Velocimetry (PIV)

In its simplest form, this technique freezes the position of a group of particles within a high-powered laser sheet, and quantifies the velocity of each droplet utilising auto or cross-correlation techniques in addition to the temporal separation between two otherwise identical pulses of radiation. Obvious sources of error include out-of-sheet motion, pixel resolution compared to droplet size and spatial separation of droplets between images. The technique is most widely used for artificially-seeded single phase flow, and difficulties have been encountered in trying to apply it to harsh spray environments[36]. However, if applicable this technique could have significant advantages over the others discussed.

3.2 DIAGNOSTIC TECHNIQUES APPLIED TO THE FLASHING JET PROBLEM

The experimental references cited from the 1960-70s utilise sampling techniques for droplet size estimation, and direct photography to quantify global spray parameters such as spray cone angle and penetration length. The measurements of Sher and Elata[37], for example, use the magnesium-oxide slide technique with post analysis for characterising sprays from pressurised aerosol canisters.

Considerable work was undertaken by the UK Nuclear industry in the 1980s considering the transportation of radioactive nuclei via airborne aerosols, for which in-house particle-sizing techniques were developed. Bates et al.[38] describe the development of a robust portable sizing analyser for field work, utilising a mixed Doppler-intensity sizing strategy for characterising superheated water-jets through sharp-edged orifices at pressures from 19-160 bar and temperatures from 110-312 °C. Limited optical access was achieved from the higher pressures (>30 bar) and higher degrees of superheat, which was attributed to the density of the spray coupled with the low-powered laser utilised (5mW).

By contrast, one of the key papers from the automotive industry (Solomon et al. (1985)[56]) utilises the diffraction methodology in the form of the Malvern Particle Analyser. Most subsequent experimental sizing investigations for flashing jets have utilised the Malvern instruments, often with compensating formulae to accommodate for the dense sprays encountered (e.g. Park and Lee[21] who use the obscuration compensation formula advocated by Dodge[39]). Directly addressing the current problem, Allen[40] utilised a modified Malvern system to characterise flashing propane releases through a 4mm final orifice (L/d = 10). Considerable modification of the Malvern based system was required to undertake measurements, and uncertainties present in the data due to the extreme optical measuring environment required involved data manipulation – obscuration levels over 90% are reported, whereas ideal conditions are around 20%. Even after analysis, it is noted that accurate droplet size distribution measurements were not possible, only gross descriptions of the variation of the droplet size within the jet. Relative droplet size distribution profiles are presented, and allow qualitative discussions of the jet characteristics. However, it is stated that quantitative accuracy requires improvement, and indicate that alternative droplet size methodologies may prove more successful.

Only one study has been found for the study of flashing jets utilising PDA, which, it is argued, would be more appropriate for the dense sprays generated by flashing jets and its ability to resolve spatially whilst provided concurrent velocity data. The EU-funded STEP[14] programme set out with the aim of addressing the problem considered in this review, and considered as an example the large-scale blow-down of a LPG release. Whilst the experimental programme appears to have been undertaken in a rigorous manner, some of the problems postulated in this review were in fact encountered in practice. The density of the spray, particularly for the larger-

scale releases, proved particularly problematic, and protection sheaths were required for the optical sections to reduce the optical density. Without these, it was claimed that PDA measurements would not have been possible. The authors found difficulty in assessing the quantitative influence of these sheaths, but estimated a 20% reduction in droplet size measurements. Under these conditions, high quality data (indicated by high data and validation rates) was collected for 2mm and 5mm releases at 7,11 and 18 bar drive pressures. The data-set is further improved by the concurrent collection of void-fraction, pressure and temperature data within the blowdown vessel. Figure 7 shows a typical droplet size distribution measured, which is a reasonably well-behaved function which could be adequately represented by a general size distribution function such as the log-normal or Rosin-Rammler distributions.

Allen[41] characterises the velocity profile across transverse downstream axial locations using a two-component TSI LDA system powered by a 4 Watt continuous wave Argon-Ion laser. Again difficulties due to harsh spray environment are reported, but after some post-processing, valid velocity data profiles across the axial centreline and several lateral profiles at various axial locations. Consistency compared with data from other pressure-liquefied studies are established, in particular the Gaussian velocity shape profile Figure 8), and self-similarity with downstream development. Interestingly, these trends are consistent with LDA data generated for effervescent atomisation (Panchagnula and Sojka, 1999)[55]. Comparison against the TRAUMA model proved relatively unsuccessful. It is concluded that LDA is appropriate for kinematic field characterisation for flashing jets, so long as care is taken in interpreting data generated.

Allen[35] also describes development of a laser-induced fluorescence technique for non-intrusive measurement of liquid-phase temperature. A particular donor was identified for use as an artificial fluorophore with liquefied propane, and found to be suitable for this and other liquefied hazardous gases such as butane. Further work was required to adapt this for free flashing jets. No direct usage as a method for quantifying relative fuel phase contributions has been reported.

It was noted in a recent unpublished study[42] of mechanical jet break-up that there appears to be a consistent discrepancy between data generated from diffraction-based instruments, and those based on phase-Doppler anemometry. Direct photography methods compared better (though not wholly satisfactorily) with the PDA data than diffraction-based systems. This serves as notice that whatever atomisation correlations are employed – and it is inevitable for the foreseeable future that empiricism will be required to provide quantitative tools - these can only be as accurate as the data sets available to validate them, and this in turn appears to depend upon which droplet sizing methodology is utilised for data generation. It is the current author's opinion that the PDA methodology is the most appropriate for characterising flashing sprays, primarily due to its better suitability to measurements in dense sprays, and the fact that its better suited to measurements at longer distances.

3.3 SUMMARY

The primary variables that require quantification in flashing jet atomisation studies are : droplet size distributions and mean droplet size, velocity components and mean velocities, relative phase distribution and jet temperature. Ideally all the diagnostics are required on a spatially resolved basis. With this specification, the most appropriate diagnostic techniques currently available are PDA (droplet size), LDA (droplet velocity components) and LIF (phase and temperature). However, the environment within a flashing jet is extremely harsh for any diagnostic technique, and hence even the most appropriate techniques will encounter some difficulties and limitations. This conclusion has been demonstrated in some recent experimental programmes undertaken by research groups experienced in obtaining measurements under harsh conditions.

4. FLASH ATOMISATION

Break up of sub-cooled jets due to pressurised release through a simple orifice is referred to as the 'mechanical break up' mode of atomisation. Atomisation due to pressurised release of superheated liquid is termed flash atomisation.

Due to the complexity of the atomisation process, so-called 'models' of atomisation are invariably correlations of appropriate dimensionless groups. Whilst non-dimensionality is the appropriate course for developing correlations with mathematical rigor, it is worth briefly discussing the physical parameters upon which atomisation is likely to be based both for mechanical and flash atomisation.

Mean droplet size (typically the Sauter Mean Diameter SMD, the droplet diameter for which the ratio of volume to surface area is identical to that for the whole spray) produced via mechanical break-up has been universally shown to be a function of exit velocity (or drive pressure), primarily due to the increase in turbulence within the jet as Reynolds number increases. Most published research has shown the droplet size to be a function of orifice size also. Hence, for mechanical break up of sub-cooled jets into standard atmospheric conditions, one would expect downstream rainout characteristics also to be a function of drive pressure and orifice size. Atomisation will be a function of the liquid parameters also, and for isothermal releases, density, viscosity and surface tension are the three parameters usually utilised. Finally, orifice geometry shape factors (typically L/d_0, where L is the length from final orifice exit to the nearest upstream expansion with the orifice, and d_0 the diameter of the exit orifice) are known to be influential in controlling the atomisation process.

As flash break-up is controlled by different phenomenological mechanisms compared with mechanical break-up (see Section 2), it is not justifiable to immediately assume the same thermofluid influences. Taking the effervescent atomiser analogy, then the performance of these atomisers is a function of drive pressure but *is relatively independent of* orifice size. They are also less dependent upon the fluid properties than the mechanical break-up process. Finally, one would obviously expect the mean droplet size to be a function of a thermodynamic quantity, the most elementary being perhaps the degree of superheat.

4.1 THERMODYNAMIC CORRELATORS FOR FLASH ATOMISATION

Before reviewing in detail the different atomisation mechanisms, it is worth listing and defining the various variables which have been proposed for use as correlators of the thermodynamic influence on atomisation. All apart from 1b, which was utilised by Park and Lee[21] are taken from Johnson and Woodward treatise (1999):

a1.	Superheat :	ΔT_{sh}	$= T_{st}-T_{sat}$
a2.	Dimensionless superheat:	ΔT_{sh}^*	$= (T_{st} - T_{sat})/(T_{sat}\,(P_{st}) - T_{sat})$
b.	Specific expansion energy	E_{exp}	$= C_{pL}\,\Delta T_{sh} + C_{pL}(T_{sat}-T_{ref})-v_{st}(P_{st}-P_a)$
c.	Specific partial expansion energy	E_p	$= \Delta h - v_{st}(P_{sat}-P_a) + v_{st}(P_{st}-P_{sat})$
d.	Approximate extended flash fraction	F_p'	$= C_{pl}\,\Delta T_{sh}/h_{fg} + v_{st}(P_{st}-P_{sat})/h_{fg}$
e.	Extended flash fraction	F_p	$= x_H + v_{st}(P_{st}-P_{sat})/h_{fg}$
f.	Jakob number	Ja	$= [C_{pL}\,\Delta T_{sh}/h_{fg}].[\rho_L/\rho_v]$
g.	Bubble growth rate	Ca	$= Ja\,(\pi\,\alpha_L)^{1/2}$

h. Droplet Weber number : $We(E_{exp}) = \rho_a d_p E_{exp}/\sigma$
(based on expansion energy)

i. Droplet Weber number : $We(E_p) = 0.5\rho_a d_p E_p/\sigma$
(based on partial expansion energy)[i]

In the above definitions, T_{st} is the upstream stagnation temperature of the liquid in containment before prior to release, T_a the temperature of the environment into which the liquid is to be released, T_{sat} the temperature of the fluid at saturated conditions at ambient pressure P_a, P_{st} the stagnation pressure, x_H the flash mass fraction at constant enthalpy, C_{pL} the specific heat of the liquid, v_{st} the specific volume at stagnation conditions, α_L the liquid thermal diffusivity (m^2/s), and σ the surface tension (N/m).

It is worth emphasising again at this stage that atomisation should not be assumed to correlate with a thermodynamic quantity alone. The dependency upon the other relevant variables (pressure, orifice-size, etc.) have to be considered also, unless there is sufficient valid evidence to assume independence. The RELEASE data reduction and analysis[7] is limited having adopted this inappropriate assumption at the onset; data from all releases are compared sequentially against one representative thermodynamic quantity. Hence, data from the release experimental programme should only be appraised against a particular thermodynamic correlator if all other influential variables remain constant i.e. an identical injector geometry, fluid and drive pressure (or exit velocity). Better correlations with the primary thermodynamic variables (e.g. superheat) may exist if the data were sorted and analysed in this manner. This action is strongly recommended to ascertain whether better representation of the 'proposed' release conditions exists.

4.2 BREAK-UP OF NON-FLASHING LIQUID JETS (MECHANICAL BREAK-UP)

The extension of traditional jet break-up mechanisms and regimes[43] to a domain involving low drive pressures and large release orifice sizes has been discussed previously by Bowen et al.[44,19] in the context of combustion hazard assessment from low pressure, high flashpoint, liquid fuel releases. Ignoring the complication induced by cavitation, the commonly-referenced jet break-up mechanisms are shown in Figure 9.

It can be seen that as the exit velocity of the jet (u_0) is systematically increased, then the jet break-up mechanism transforms from the famous Rayleigh-type instabilities[45], to shear-induced atomisation, comprising first-wind, second-wind and finally full atomisation. So-called fully atomised sprays are characterised by their very small break-up length (represented by L_B in Figure 9). Generally, characteristic droplet sizes decrease as the jet velocity increases, i.e. traversing the various jet break-up modes. Numerous correlations involving the various control variables (primarily exit velocity, orifice size, and fluid properties) have been proposed for the downstream atomisation process[13,46,47]. Recent work[19] has indicated that correlations for high-pressure diesel-type injectors may also provide similar predictions to those from correlations for low-pressure, larger orifice releases, i.e. the physics governing the jet break-up processes may scale reasonably well. Although not rigorously established yet, this is worth noting in terms of development of methods for quantifying flashing jet atomisation, where it is more appropriate to develop basic physical correlations in small-scale experimental programmes. Scaling can be appraised then as a separate verification programme, with a reduced test programme (as a model is being verified rather than developed) and hence cost.

[i] The formula $We(E_p) = 0.5\rho_a d_p E_p/\sigma$ quoted by Johnson and Woodward appears to be inconsistent with the formula for $We(E_{exp}) = \rho_a d_p E_{exp}/\sigma$.

Generally, the SMD for sprays produced from this type of jet break-up is reported to show a positive correlation with orifice size (SMD $\propto d_0^a$, where '$\propto$' means 'proportional to' and where the exponent 'a' varies between 0.262 and 1.2), and inverse correlation with liquid pressure (SMD $\propto \Delta P^b$, where the exponent 'b' varies between –0.07 and –0.69, and $\Delta P = P_o - P_a$ is the pressure change across the orifice to ambient). Hence, in terms of dispersion calculations for liquid rainout, and idealising by ignoring dispersion heat and mass transfer at this stage, one would expect rainout to show a positive correlation with increase in orifice size due to the larger droplets produced during the atomisation processes. Similarly, for mechanical break-up, an inverse correlation for rainout with drive pressure should be anticipated, which as discussed later, has in fact been indicated in large-scale experiments also[9,17].

All atmospheric dispersion codes currently appear to adopt the critical Weber number criterion – $We_{crit} = \rho_a . u_0^2 d_p / \sigma_L = 10\text{-}20$ - to estimate maximum sizes for stable droplets from mechanical break-up. Whilst appropriate for single droplet situations – these types of correlations have been used to determine whether explosions can break down large droplets from water sprays, for example - this methodology is not considered appropriate as a correlator of mean droplet size for this application; it is independent of orifice size, and the exponent of drive pressure is outside the range measured by all other researchers (an exponent 'b' of –1.0).

On the basis that there seems to be little experimental verification of the hypothesis that this single droplet break-up criteria can be extrapolated to quantify the mean of an ensemble of droplets, the critical Weber number approach to characterising mean droplet sizes produced via mechanical break-up is not endorsed. An analogous situation has arisen in the study of the related problem of spray impingement, where initial modelling attempts employed summation of single droplet-impingement studies, whereas it has now been shown that this approach is also inappropriate[46].

Furthermore, whilst the critical Weber number approach may prove useful to bound the maximum droplet size possible from a particular release scenario, empirical spray correlations provide an additional benefit in that it has been proposed to use the SMD as a basis to derive spray distributions via appropriate spray distribution functions such as the Rosin-Rammler, as discussed later on in this section.

A recent HSE study[19] investigating conditions under which mechanical break-up of high-flashpoint liquid fuels induces a hazardous flammable atmosphere, proposes an empirical relationship between the dimensionless SMD and the jet Weber number ($We_J = \rho_L u_o^2 d_o / \sigma_L$) and jet Reynolds number ($Re_J = \rho_L u_o d_o / \mu_L$) for 'large'-orifice, 'low'-pressure releases. However, only liquid drive pressure differential $P_o - P_a$ and exit orifice size d_o were systematically varied, as the emphasis of the correlation was to provide trends and likelihood of a flammability hazard being realised, rather than to provide a source term for detailed post-spray calculations as required for this two-phase dispersion problem. Other influential characteristics such as orifice length-to-diameter ratio L/d_o, surface roughness, downstream distance and the influence of liquid properties were not considered. Hence, it is *strongly recommended* that the correlation (2) be updated accordingly before being utilised in atmospheric dispersion models, where sensitivity to initial spray conditions are likely to be critical. Such correlations for jet breakup for a particular fluid are usually expressed in the following non-dimensionalised generic form :

$$\frac{SMD}{d_o} = F\left(We, \mathrm{Re}, \frac{L}{d_o}\right) \qquad \textbf{(1)}$$

where d_o is the orifice diameter and We and Re are appropriate Weber and Reynolds numbers respectively. To generalise this correlation further for application to different fuels, the relevant

liquid properties need to be included in this correlation, also in appropriate non-dimensional form. The function F is usually adequately represented by power-law relationships, and for the large-orifice low-pressure data, the following non-dimensional form provides the best correlation of the data :

$$\frac{SMD}{d_o} = 82.23\, C_D^{\,0.64}\, We_J^{\,-0.07}\, \mathrm{Re}_J^{\,-0.5} \qquad (2)$$

where the fluid variables in the jet Weber and Reynolds numbers – indicated by the subscript 'J' - have been taken to be those relating to the liquid properties, i.e. water. These parameters have been simply used as part of the non-dimensionalisation process to produce a mathematically consistent equation, and as indicated earlier, should not be considered as an indication of suitability for use in providing predictions for other liquid releases.

Assuming a discharge-coefficient relation between release pressure and exit velocity, it is simply to show that the above correlation provides an inverse relationship between SMD and release pressure (with exponent –0.32), and increase in SMD with increase in exit orifice size (with exponent 0.43). These exponents are within the ranges reported by previous researchers for pressurised releases through simple orifices, but under different release conditions, and this provides some confidence in the form of the correlation, notwithstanding the known deficiencies.

It has been noted that there is a considerable spread of data generated from different types of droplet-sizing laser diagnostic equipment. Each technique has inherent inaccuracies as noted in the previous chapter, and comparison between results from the various droplet sizing techniques is a difficult proposition. However, clearly care is required when comparing data and deriving trustworthy empirical models.

Recent work in this area at Cardiff has considered the influence of L/d_0 ratio with particular interest in cavitation[42]. Results have shown, consistent with other workers, how important orifice length is for subcooled jets, and this parameter is likely to become even more influential once superheat is introduced due to its influence on the two-phase flow structure upstream of the exit.

As an indication of the magnitude of the deviation in droplet size for fully flashing releases – i.e. high superheat - from the mechanical break-up prediction, Figure 10 shows the prediction purely from mechanical break-up using correlation 2 (modified somewhat to provide some account of variation of liquid properties), compared with a sample of the data measured in two previous large-scale experimental characterisation programmes. It is suggested that the analogy between mechanical breakup of sprays and atomisation of sprays under low superheat conditions should be modified to take account of the vapour produced during the flash – the flash fraction – that is, the size of the droplets should reduce to account for the volume of vapour produced. Sample calculations have shown that generally this modification is only likely to change the size prediction slightly, and certainly would not account for the large differences indicated in Figure 10 between mechanical breakup and flashing under high superheat conditions. This minor modification to the mechanical breakup analogy is also indicated via rainout in the useful schematic provided by Muralidur et al.[17] in Figure 11, identified by the gradual decline in rainout as the degree of superheat is increased up until the transition to flash atomisation conditions is attained.

Concerning the distribution of droplet sizes within the spray, Elkobt[13] suggests that spray distributions from simple orifices could be adequately represented by a Rosin-Rammler

distribution. Note it does not immediately follow that a self-similar droplet distribution should be maintained further downstream after heat and mass have been transferred. This is the recommended distribution for use at this stage of development in characterising droplet distributions from jets under mechanical break-up, as there is implicitly some experimental validation. A detailed analysis of whether the log-normal or any other distribution would in fact represent these types of sprays better than the Rosin-Rammler has not be undertaken. Though this comparison would be relatively straightforward, the spray distribution is considered of secondary importance at this stage of development in light of the lack of confidence in predicting the mean droplet diameter. Different forms of distribution functions may be obtained from standard atomisation references [24], the one advocated by Eltkobt[13] expressed conveniently in terms of the spray SMD in the following format :

$$1 - v(d_p) = e^{-0.422\left(\frac{d_p}{SMD}\right)^{5.32}} \quad (3)$$

Here, the function $v(d_p)$ represents the fraction of the total volume of spray contained in droplets of size less than d_p, and provides a useful first approximation for atmospheric dispersion releases.

More recent developments of sub-models of atomisation for automotive applications has seen the introduction of the so-called 'blob' models, first advocated by Reitz[47]. This subdivides the overall atomisation process into primary atomisation where large droplets are sheared from the jet surface, followed potentially by aerodynamic break-up of the primary droplets into secondary spray. The primary spray is modelled by imposing axi-symmetric disturbances onto the steady jet. This wave-like disturbance is then fed into the conservation equations to derive the dispersion equation for the temporal frequency of the instabilities. This equation may be solved to derive the wavelength associated with the most likely surface wave, which in turn is linearly related to the size of droplets created from parent 'blobs' of larger size. The rate of change of parent droplets is inversely proportional to the break-up time. Whilst it may be possible for this type of model to be introduced into atmospheric dispersion models, this is not recommended at this stage of development as the required diagnostic may be equally well obtained using direct correlations without the additional computational overhead.

The first step towards validating the UDM code for superheated releases should be to compare a sub-cooled release of liquid against existing data sets[7] using the new mechanical break-up correlation to check that the dynamic processes are performing satisfactorily. A sensitivity study could then be undertaken to investigate the effect of mean spray size and droplet distribution characteristics on rainout prediction. Water would be the obvious test fluid, with care taken over the influence of atmospheric humidity. Clearly one needs to be sure that the dynamics of the system can be predicted before one develops a model to include the further complication represented by the thermodynamic aspects.

4.3 BREAK-UP AND ATOMISATION OF FLASHING JETS

Various authors[48,49] have reported little or no discernible difference between jet releases under 'low' superheat conditions compared with mechanical break-up. Moreover, other authors have reported different modes of flashing atomisation, ranging from expansion and catastrophic disintegration of bubbles developing outside the exit orifice, to development of vapour upstream of the exit orifice. Hence, these different phenomena are divided into appropriate sections, with criteria governing transition between the various modes reported where such correlations are available. Generally the mean size of droplets produced via atomisation decreases as the degree of superheat increases.

4.3.1 Low Superheat

Earliest studies of flashing jets were limited to jets with relatively low degrees of superheat. Under these conditions, the effect of nucleation appears either to be negligible, so that mechanical jet break-up prevails, or restricted to the external break-up mode where bubbles are generated and grow within the jet downstream of the exit orifice. This may be represented schematically as shown in Figure 11[18]. Hence, it can be seen that from the perspective of jet break-up, flashing atomisation appears to be limited by a transition superheat limit, allowing mechanical break-up mechanisms to dominate into the superheated region (N.B. the terminology has been modified compared to that used by Muralidhar et al.[18], so that 'transition' superheat is now used instead of 'critical' superheat as the word critical has specific implications in association with phase change which may be cause of unnecessary confusion. The categorisation of degree of superheat has to be tempered by the influence of L/d_o ratio, which itself can induce significant changes in atomisation regime.

As many atmospheric dispersion scenarios envisaged consider relatively low pressure releases through large orifices, then large droplets (SMD of 100s microns) would be generated via mechanical break-up mechanisms, with correspondingly large rainout fractions. Moreover, as noted earlier the correlations developed for mechanical break-up predict that a positive correlation with orifice diameter should be expected, and inverse correlation with release pressure.

Whilst the Hydrogen Fluoride (HF) data presented by Muralidhar[18] is complicated by some complex aerosol chemistry, it is worth noting that both the pressure and orifice diameter trends from mechanical break-up are consistent with their rainout data. The authors argue strongly that their releases did not show any signs of flashing, and so it appears that mechanical break-up would indeed be the most appropriate model for the atomisation under these 'low' superheat conditions. Hence, subject to the issues of complex chemistry, this HF data may well represent a substantial data set of liquid releases of relevance under low superheat, allowing the mechanical break-up mechanism to dominate, and as such, represents a verification data set for an atmospheric dispersion code such as UDM typical of low superheat conditions[ii].

The authors claim that further improvements on an already good agreement between model predictions and data could be achieved if a better atomisation model were introduced for mechanical break-up, and if relative motion between droplets and the jet fog could be introduced. Both these suggestions could be relatively easily incorporated into a model such as UDM to provide a second logical step towards appraisal of the UDM modelling methodology in terms of predicting rain-out.

A final note regarding conditions of low degrees of superheat is a corollary from the discussion above, which has been confirmed by other independent studies[50]. Superheat degree does not correlate with the atomisation process at low superheat. There is also evidence from the data generated from the controversial methodology of deriving droplet diameters by back-calculations as presented in Woodward and Johnson[7] – see their figure 4. This data should be represented in light of a transitional superheat – where a strong correlation begins – and grouped for data points where all other variables (orifice size, pressure, fluid, etc.) remain constant. Here, it is recommended that for the 'low-superheat' condition, the correlation used for predicting droplet characteristics of a sub-cooled atomising jet as discussed in section 4.2 be utilised.

[ii] This would require further extension of the thermodynamic formulation in the UDM to allow for droplet modelling of multi-compound mixtures including HF.

Clearly to progress further towards a quantitative methodology, valid criteria governing transition between mechanical and flashing break up need to be established. Kitamura et al.[49] propose a transitional correlation using superheated water and ethanol flowing through 'long' nozzles ($50 < L/d_o < 115$) and flashing into an evacuated chamber. Their correlation is claimed to govern transition to 'complete' flashing; they compare favourably with the earlier data-set of Brown and York[48], where flashing into an atmospheric environment was studied. Notwithstanding the requirement for further validation and generalisation, this correlation provides a useful benchmark against which current data-sets and modelling sensitivity studies can be appraised:

$$\left[1.0 - e^{-2300\frac{\rho_v}{\rho_L}}\right] Ja = 100\ We^{-1/7} \qquad (4)$$

where Ja is the Jacob number (see Section 4.1), We is the Weber number ($We=\rho_a u_0^2 d_p/\sigma_L$ - a measure of relative influence of inertial versus surface tension forces), ρ_v the vapour density and ρ_L the liquid density. Figure 12 shows this correlation compared with some representative release examples. This correlation should be appraised against the albeit limited data set for proposed application in atmospheric dispersion models.

4.3.2 'External' Flashing Atomisation Mode – 'Intermediate' Superheat

At slightly higher degrees of superheat (or longer L/d_o ratio), the mechanical break-up process no longer dominates. Bubbles are observed to develop within the liquid jet outside the nozzle after a relatively long 'idle' period (nucleation), but after which they grow rapidly to shatter the jet. Based on this phenomenological description, one would expect this mode of atomisation to dominate over mechanical break-up, especially under low pressures (<10 bar) and relatively large orifices (>1mm) where mechanical break-up induces large droplet sizes. Hence, one would anticipate correlations between atomisation and degree of superheat - or other appropriate thermodynamic measure - to exist.

Models have been published for jet break-up due to bubble growth in the external mode:

- Lienard and Day[51] developed a general formula for the jet break-up criterion. The model was essentially based on a characteristic break-up time, which is the sum of the idle time and the time for the bubble to grow as large as the initial jet diameter.
- Orza and Sinnamon[52] (1983, 1984) assumed jet break-up when the bubble radius grows twice as large as its initial radius.
- Razzaghi (1989)[62] considered the mechanical and bubble-bursting break-up mechanisms to occur in sequence, the liquid jet breaking up into relatively large droplets before micro-explosions create smaller droplets.
- Recently, Zeng and Lee (2000)[53] have developed the so-called 'blob' model first proposed by Reitz and Diwakar (1986)[54] for mechanical break-up to include the effects of expanding bubbles due to flashing. This flashing model is then integrated with a well-known CFD model developed specifically for engine applications (KIVA).

Hence, whilst models actually exist and are of a form suitable for integration within a larger more general numerical code, they are not as trivially implemented as would be a one-equation correlation of similar form to that proposed for mechanical break-up. For integration within atmospheric dispersion codes, it is assumed that single correlations are most appropriate if they exist.

4.3.3 Internal Flashing Mode – 'Effervescence due to Superheat'

This mode of atomisation is the most catastrophic, and the one envisaged to have strong phenomenological links with effervescent atomisation phenomenology. It is capable of producing very fine sprays indeed, which would result in low or zero rainout. The internal flashing mode may itself may be subdivided into various subsections, as shown in the earlier section 2.3. The prevailing conditions are consistent with those studied experimentally at large-scale by the UK HSE[40,41] and in the EU STEP programme[14]. Moreover, controlled experimental releases for which no rainout has been recorded are considered (by the first author) most likely to have atomised via this mode.[iii]

The atomisation process itself is strongly dependent upon the two-phase flow development within the nozzle – or approach to the final exit orifice - in an accidental release, and Figure 6 indicate the various stages of flow development within the nozzle prior to release into the atmosphere. Effervescent atomisation has recently indicated[22,55] that a transition in internal flow regime is also accompanied by a transition in mode of atomisation. From flow of superheat liquids in pipes, it is now well established that the two-phase effluent is induced via two mechanisms: homogeneous and heterogeneous nucleation.

For prediction of droplet sizes outside the nozzle, then parameters required within the nozzle upon which atomisation strategies can be developed need to be defined. It seems reasonable to presume that transition criteria between each of the internal flow modes shown in Figure 3 – bubbly, slug, annular, etc. – at the time of exiting the orifice is required. Recently this has been shown under isothermal effervescence to be a function of mass air-to-liquid ratio[iv] (ALR) - or the void fraction, ε. Whether this is universally true is not clear at this stage. Extending this analogy to flashing flow, then it is known that these modes can develop along the length of a pipe or tube in heat transfer applications (Figure 6). Hence, the mode of flow will be a function of time in a Lagrangian sense, or equivalently a function of position along the pipe (hence the reference to L/d_0 dependence in experimental studies).

Hence, it is suggested that the information required at the exit orifice for a flashing release in order to correlate downstream spray characteristics are void fraction (or ALR), flow state (bubbly, annular, droplet-dispersed, etc.) and discharge pressure. The void fraction and flow state will be dependent upon the primary input parameters such as degree of superheat and geometrical dimensions. It may be that this spray dependence can be reduced further to two parameters, if there exists a unique dependence between void fraction and flow state. This is currently not clear, however, and should be considered in future studies. Hence, a model that predicts the void fraction (or ALR) at the nozzle exit is recommended for the development of a rigorous flash atomisation model, and as discussed earlier[iii], these types of models have already been proposed albeit for limiting cases.

[iii] This is inconsistent with most modelling attempts for these data-sets, where no upstream vapour generation has been considered by virtue of the relatively small length of pipe utilised in the experimental programmes. For example PHAST assumes atmospheric expansion from liquid to two-phase only, except for very long pipelines where 1D homogeneous pipe flow modelling is applied and two-phase to two-phase expansion is assumed. Thus the discharge models are limited to the extreme cases representing very long pipelines, or very short pipes. However, the majority of scenarios are likely to lie in the domain between these two extremes, and so predictions regarding the flow state in this intermediate state of practical relevance have not been employed as yet.

[iv] Note that the ALR or the void fraction equals the air-to-liquid ratio for non-flashing liquids only. Otherwise it equals the vapour-to-liquid ratio.

Hence, for a systematic atomisation model in the 'high superheat' region, it is proposed that ideally a model is required which predicts the various flow states outlined in Section 2 at the exit. Empirical atomisation models would then be based upon exiting flow state rather than more primitive upstream thermodynamic variables, and it may well be possible to utilise the various atomisation models proposed in the literature for various two-phase flows directly (e.g. effervescent models for bubbly and bubbly-slug flow suggested here, and liquid-film atomisation models for higher void fractions as suggested previously[56]).

In light of this discussion, it was decided appropriate to review the literature pertaining to modelling the development of two-phase flow state within pipes when nuclei creation and bubble growth is realised, before reviewing attempts to provide direct correlations.

Flow regimes within pipes and tubes under flashing conditions

Several workers have considered the prediction of changes in flow-state in nucleating or boiling flows, primarily due to the interest of such flow in heat exchangers within the nuclear industry, for example. Jones and co-workers[57,58] have developed a series of simple 1-dimensional numerical models, initially considering heterogeneous nucleation[57] but more recently for the more realistic application of mixed nucleation[58].

Saha et al.[59] presented a semi-empirical approach to the development of two-phase flashing regimes along a pipe. All established flow modes are considered, and simplified modelling is introduced at each stage. The void fractions corresponding to transition between the bubbly, bubbly-slug and annular/annular-mist were assumed to be $\varepsilon_{b,max} = 0.3$ $\varepsilon_{b,max}=0.8$ and $\varepsilon_{b,max}= 0.95$. These values seem fairly representative and consistent throughout this literature. A further zone is added to represent the point of flashing inception and bubble nucleation (ε_0). The established understanding of a critical nucleated bubble size governing growth is then adopted, where the critical size is determined by the competition between expansion due to the vapour pressure and the restraint to this offered by the surface tension force at the liquid/vapour interface. The limit of bubble inception is then derived from the critical inception bubble size and the bubble number density at the flashing inception point. The latter variable was employed as a parameter of the model and was 'tuned' to various data sets provided.

All further nucleation downstream is neglected on the basis that bubble growth rate is a strong function of development time. An equivalent radius is presumed for non-spherical bubbles, and a simplified model for the relative velocity between the bubbles and the liquid. Void fraction is suggested as the correlating parameter for the thermodynamic aspects of atomisation via the internal flashing mode, though this can be readily converted to a parameter more commonly utilised in atomisation technology, the mass air-to-liquid ratio. An 1-D axial marching technique was employed to predict void fraction as a function of downstream distance, and this was compared against experimental data. Reasonably good agreement of the void fraction was observed subject to the aforementioned 'tuning' of the number of bubbles at inception.

The above type of method for calculating the void fraction within the pipe could be coupled with an empirical atomisation model based on the two-phase flow characteristic at the orifice exit plane. This would then form one module within the overall consequence calculations[v]. Aside from the bubble number at inception which is an independent parameter in the flow models discussed so far, the other input variables would be the primary input parameters of the release : thermo-fluid dynamic state, orifice design and fluid properties. The bubble number

[v] In the consequence modelling package PHAST, the UDM dispersion model starts from the post-expansion conditions, with the expansion calculations carried out by the ATEX model. The ATEX model allows for two-phase to two-phase expansion, where the pre-expansion void fraction could be provided from flashing calculations carried out by a (long) pipeline model.

density at inception could be provided as an empirical correlation if no more rigorous methodology could be found.

Blinkov et al.[58] developed this approach further, and again based their model on the prediction of void fraction to differentiate flow regimes. An interesting note arising from all these series of papers is that no nucleation is observed upstream of the throat in a convergent-divergent nozzle, and the widespread use of this parameter in distinguishing transition between different two-phase flow regimes.

Again to emphasise the relevance to the atmospheric dispersion work, the effervescent atomiser studies have demonstrated how critical the two-phase flow conditions (via ALR) is on atomisation quality downstream, and hence the justification in concentrating on prediction of the void fraction within the orifice.

A physical explanation of the $\varepsilon = 0.3$ limit for bubble-slug flow transition is provided by Ishii and Mashima[60] (1983), who show that this is the limiting condition before spherical bubbles touch. The same critical void fractions for flow transition used by Saha et al.[59] were employed, and the model is developed for bubbly and bubbly-slug regimes only ($\varepsilon < 0.8$). Independent models previously developed by the authors are introduced for heterogeneous and homogeneous flow respectively. Hence the integrated model provides source term model from both sources, and in this sense is a development of the earlier models.

Mathematically the model is essentially a 1-D 5-equation mechanical equilibrium (no phase-slip), thermal non-equilibrium model providing vapour generation from heterogeneous and homogeneous nucleation. Semi-implicit methods were used for differencing within the numerical scheme, but the model was capable of running on 32 bit HP microcomputer 9816 running at less than 16 MHz.

The model predictions were compared against various sources of data in the literature and it was shown that a model based purely on the bubbly-flow phenomenon only compares well against the experimental data up to void fractions of about 0.35. Thereafter, the models representing other flow regimes diverge such that differences of about 15% between models are identified for void fractions of about 0.6. The model including bubbly, bubbly-slug, transitional and dispersed flows shows remarkable agreement with data, with errors in void fraction typically within about 5% at a particular axial distance downstream of the throat.

An important development with regard to integrating internal two-phase flow structure within the nozzle to the external atomisation process is noted in the paper of Fujimoto et al. (1994)[61] for the application of automotive fuel injection. The approach adopted appears to be consistent with that advocated within this report, i.e. the internal flow structure is predicted by the primary input variables providing the secondary input variables of void fraction and pressure at the orifice, which are then used to correlate downstream atomisation characteristics. In this work, superheated conditions are achieved by varying the back pressure, as discussed in Section 2 and represented in Figure 2.

Whilst the approach previously proposed by Saha et al.[59] is adopted, in this paper the only remaining outstanding parameter from this previous model – the number density (N) of bubble nuclei – is proposed as an empirical function of degree of superheat (this function will be nozzle specific, so is likely to have to be generalised). This provides an excellent benchmark and allows a model to be constructed for void fraction at the orifice depending only upon the input variables of the global dispersion problem. The number of incipient bubbles at nucleation is proposed to bear exponential relationship with superheat, assuming the specific form for the problem considered :

$$N = 5.757 \times 10^{12} \exp(-5.279/\Delta T_{sh})$$

The overall model for the flash droplet formation process through a pintle injector is presented in Figure 13[61]. Predictions are provided for superheated n-pentane and n-hexane. Of course only mono-disperse droplet quality is predicted due to the nature of the model, so results are compared with the arithmetic mean from a limited data set, where reasonable agreement was observed. Nevertheless, it has been demonstrated that the methodology proposed within this report of correlating the atomisation process to the two-phase flow structure at the exit orifice is plausible.

Global droplet-size correlations for flash atomisation

Droplet size correlations were first proposed by Brown and York[48] for superheated jets (water and Freon) at release pressures between 5-10 bar. Micro-photography was used to measure droplet distributions and droplet velocity - similar to the PIV methodology. A log-normal fit to the size distributions was considered appropriate. The data from superheated water jets could be correlated by an equation linear for the d_{10} volume undersize with respect to injection water temperature whilst inversely proportional to the droplet Weber number :

$$d_{10} = [1840 - 5.18\ T\ (°F)]/We$$

Although not dimensionally correct, this correlation does represent the influence of both thermodynamics (via the temperature) and fluid dynamics (via the Weber number), and so simply from the viewpoint of the processes represented in the functional relationship, this correlation seems creditable.

The model of Sher and Elata[37] propose that the droplet size produced during flash atomisation is linearly proportional to liquid surface tension, and inversely proportional to the superheat degree. Their model is based on nuclei generation and a bubble bursting mechanism. There are some problems with applying the final correlation proposed for droplet size with any generality:

- The authors claim the source of vapour nuclei was a valve within their injection mechanism (specific to aerosol deodorant containers). Without this, nuclei were not generated, although the parameter representing the volume density of vapour nuclei could presumably be modified for a more general case.
- Secondly, the analysis was undertaken for binary mixtures (toluene and Freon 22) so it is not clear how this would differ for single component mixtures, though again presumably similar physical processes take place and parameters could be modified accordingly.

Solomon et al.[56] subdivide the release conditions analogous to the approach advocated in this document, and propose 4 correlations, the first due to pure mechanical break-up, which has already been discussed in depth in Section 4.3.1, developing through to internal flashing, for which a correlation analogous to that recommended for a pre-filming type air-blast atomiser is suggested:

$$\eta_n\ SMD/(1+m_L/m_v) = 0.073\ [\ \sigma_L/(\rho_v u_v^2)]^{0.6}[\rho_L/\rho_v]^{0.1}\ d_o^{0.4} + 6.10^{-4}[u_L^2 d_o/\sigma_L\ \rho_v]^{0.5}$$

Hence, this work provides some support for the proposal presented here of utilising analogies between flash atomisation and specific categories of atomisers. However, here it is argued that the effervescent analogy is a better representation of conditions pertaining within the orifice during internal-mode atomisation, compared with the prefilming atomiser, especially under conditions of bubbly-flow; note effervescent atomiser technology had not been discovered in

1985. The pre-filming atomiser is likely to perform best at very high degrees of superheat when the void fraction is of the order of 0.9 or greater.

Solomon et al.[56] demonstrate that flashing break-up reduces mean droplet size compared to mechanical break-up mechanisms. d_{50} mean droplet sizes measured using a magnesium-oxide impact methodology indicated variations between 30 and 90 μm depending upon release pressure (2-6 bar), temperature (15-60 C) and percentage of propellant within the mixture.

Razzaghi (1989)[62] employs an external flashing model to water jets at high pressure (> 100bar) and high degree of superheat (>475 K initial temperature), although under these conditions, one would presume a strong likelihood of internal nucleation. Hence, it may be that this model is more representative of the external-flashing mode introduced and described in Section 4.3.2 of this report.

The model presumes that droplets are sheared from the jet before the vapour generation takes place within spherical bubbles. The critical Weber number approach is utilised to estimate the primary droplet size, which is then extended to develop a log-normal distribution of droplet sizes. Secondary (tertiary) droplets originate from the shattering of the bubbles within droplets, and are estimated to give rise to between 1-10 droplets per bubble; size is then determined from mass conservation. A critical superheat transition is identified, below which mechanical break-up dominates, and superheat only serves to enhance droplet surface evaporation. For 50 bar water releases at 590 K initial temperature droplet sizes less than 25μm are predicted. The author does concede in conclusion that alternative approaches to the droplet-bubble external atomisation model are possible.

Senda et al.[63] present data for flashing n-Pentane and n-Hexane jets at pressures of less than 10 bar. Droplet size distributions are measured using micrograph photography. Flashing is realised by reducing the chamber pressure, as discussed in Section 2. Mechanical break-up dominates under sub-cooled conditions, with mean droplet sizes typical of mechanical break-up (several hundred microns) prevailing. When slightly supersaturated conditions are encountered, there is a marked increase in SMD. The authors claim this to be due to the contracting spray; a contracting spray in this situation seems non-intuitive as conventionally cone-angle increases with decrease in ambient pressure for pressure atomisers. Flashing jets are also known to substantially increase cone angle of course, though flashing atomisation is unlikely to have commenced at this stage. This may be a spurious anomaly or true difference between the presumed equivalence of mechanical break-up for sub-cooled and low superheat jets which requires further investigation. Further reduction in the chamber pressure is accompanied by a sharp decrease in droplet SMD associated with flashing atomisation. SMDs of the order of 60 μm are achieved for a drive pressure of only 2.5 bar when the pressure difference between chamber and liquid vapour pressure is –0.3 bar. It is noted that the flashing spray is far more uniform than the spray formed by mechanical break-up, with uniformity along radial profiles also. This is consistent with most other research and again helpful in proposing simplified modelling approaches.

Park and Lee[21] show that the variation of SMD across a transverse spray diameter decreased with increase in superheat – the radial distribution became more uniform – whilst the mean SMD also increased with increase in superheat consistent with all previous studies. 50mm downstream of the exit orifice, the mean (averaged across a spray-radius) SMD decreased exponentially with increasing dimensionless superheat (ΔT^*). Release conditions of this data set (2-4 bar; 10-30 C superheat) appear very similar to some of the tests in the CCPS rain-out data-set for water, and it would be a useful benchmark to take this data set as input for the appraisal of dispersion calculations downstream in terms of rainout, assuming a scaling law for the flash atomisation process.

Johnson and Woodward[7] reference other suggestions proposed for calculating spray quality of flashing jets. As well as some of those already mentioned, they include the correlation of Crowe and Comfort (1978)[64]:

$$d_p = 4.6\left[\frac{\sigma\, k_L\, d_o}{u_o\, \rho_L\, C_{pL}\, \Delta P}\right]^{1/3}$$

and an expression derived by Koestel et al. (1980) for predicting minimum drop size, which includes a term to correlate the point at which flashing break-up occurs, indicated to be of the order 0.07-0.1 for 0.02-0.04 inch pipes. As examples, liquefied propane would be predicted to flash below 30° C and water at around 40° C. Whilst the minimum droplet size equation would provide useful information regarding spray characteristics if fully validated, of course information on the spread or mean droplet size would be required to be suitable for predicting rainout satisfactorily.

Finally, Nagai et al.[65] developed a series of very promising correlations which change form according to L/d_o ratio. The influence of superheat – via the dimensionless superheat, ΔT_{sh}* - is also considered, as well as orifice diameter. Rather neatly, the influence of the injection pressure is shown to be accounted for in the dimensionless superheat expression; it changes the denominator term via its corresponding saturated temperature. These correlations should certainly be appraised as a priority in future development work, as they certainly appear to have considered the primary variables influencing the atomisation process. The authors certainly consider the various transitions in flow structure occuring as the control parameters are systematically varied. Droplet size distributions are also given some consideration, and represented by a Nukiyama-Tanasawa distribution. It is also shown that the absolute maximum droplet size measured in the spray varied as a multiple of the SMD with a multiplication factor ranging from 2.0-2.6. This is somewhat higher than the 1.8 quoted by Eltkobt[13] for reference to mechanical breakup.

Other points to note concerning this work are that the particle sizing was undertaken using an intrusive impactor methodology with post-analysis, and hence should be reappraised using more mature laser diagnostic techniques. Secondly, the correlations proposed are specifically for brass nozzles, though the authors provide data and note differences in atomisation quality with change in nozzle construction material due to surface roughness and wetness influencing the number of nucleation sites.

The equations take the following form[vi]

$$SMD = 36.8\left(\Delta T_{sh}{}^{*}\right)^{-2.58} \quad microns \quad , \quad for \;\; L/d_o < 7 \;\; and \;\; 0.55 < \Delta T_{sh}{}^{*} < 1.0$$

for the shorter nozzles ($L/d_o < 7$) , and

[vi] Note that no correlation was provided for smaller nozzles in conjuctions with small superheat. There is also an unexplained gap between $L/d_o = 7$ and $L/d_o = 7.8$.

$$SMD = 70.4 \left[-1 + 0.14 \left(\frac{L}{d_o} \right) \right]^{-0.22} d_o^{0.72} \left(\Delta T_{sh}^{*} \right)^{-0.38} \quad microns \;, \quad L/D > 7.8 \quad and \quad 0 < \Delta T_{sh}^{*} < 0.55$$

$$SMD = 39.1 \left[-1 + 0.14 \left(\frac{L}{d_o} \right) \right]^{-0.22} d_o^{0.72} \left(\Delta T_{sh}^{*} \right)^{-1.33} \quad microns \;, \quad L/D > 7.8 \quad and \quad 0.55 < \Delta T_{sh}^{*} < 1.0$$

for the longer nozzles.

4.3.4 Relevant Recent Large-scale Studies, Models and Reviews

As noted in the introduction, several large scale studies and reviews directly considering the theme of this report have been published over the last 10 years. These include the treatise of CCPS studies by Johnson and Woodward[7] which was subsequently reviewed in the UK by AEA[9] on behalf of the Health and Safety Executive, and briefly by DNV (Webber[66]). Another programme of work was undertaken by the Health and Safety Laboratory[35,40,41] and an EU initiative under the so-called STEP programme, undertaken by CEA-Grenoble[14,15].

CCPS book by Johnson and Woodward: CCPS experiments and RELEASE model

Johnson and Woodward[7] collate and review a series of large-scale experimental programmes started in the 1980s and relevant literature studies with the aim of proposing a validated model for prediction of rainout from flashing jet releases. Each large-scale programme is described briefly, and the raw data plus relevant derivative variables presented in a useful summary tabular format. Some of the data is processed by the authors in an attempt to accommodate the effects of re-evaporation from pools created by rainout. Reviews of relevant aerosol and flashing technology are included.

In the overall RELEASE model, the sub-model applied for atomisation is the common critical Weber number method, with a modification of the characteristic velocity as the difference between the expansion and discharge velocities for the case of the flashing jet. The velocity term includes two-phase parameters which is credible in the sense that some influence of the two-phase flow is attempted, but still the overall methodology relies on the basic process being a competition between inertial and surface tension forces. In all runs reported, a fixed value for the bubble-constant is adopted. Utilising the atomisation sub-model, the authors show that mechanical break-up always dominates flash break-up, which is considered a major inconsistency compared with experimental evidence in the literature. Other models are referenced which do not result in this conclusion, but unfortunately no form of comparative study is offered. Rainout is determined when droplet trajectories exceed that of the cloud boundary in an analogous way to other models (TRAUMA[10]), with settling velocity determined by equating forces in the usual way.

RELEASE predicts 100% rainout for low superheat due to the lack of evaporation modelling during rainout. Whilst for high boiling-point liquids such as water 100% rainout is realistic, for more volatile substances (e.g. CFC-11) this leads to considerable error. By contrast, at higher values of superheat the model agrees better with the corrected data for the volatile substance than water, a rapid decrease in the rainout efficiency being predicted which is not noted in the corrected data. Further manipulation of the experimental data is attempted to improve the agreement and accommodate for the lack of evaporation in the model. This serves to emphasise the obvious statement that any dispersion model requires droplet evaporation to enable reasonable agreement between data and predictions. It is extremely important to note at this stage that the authors have not presented the CCPS data in a way that allows variation and comparison of one influential variable at a time. This becomes even more critical in the final

section of the reference where correlations are proposed based on 'reverse modelling', i.e. utilising an atmospheric dispersion model to iterate between estimated initial droplet size (as this is not measured) and the measured rainout fraction for each test case. Whilst it could be argued that this approach is reasonable in a data reduction and interpretation exercise, it has obvious shortcomings if it is to be used to generate atomisation models. First, the atomisation model is then clearly wholly reliant on the accuracy of upstream submodels such as those modelling discharge rates, droplet heat and mass transfer, etc. Moreover, the accuracy of the rainout data, which in this case is known to have inherent deficiencies, also has a direct bearing on the atomisation model so derived.

The reverse modelling approach is certainly open to criticism for its lack of scientific rigor. However, it does serve a purpose in that it can provide a relative measure of change in droplet size inferred from the CCPS data, and without measured droplet sizes at source for any of the data, this is the only option available other than rerunning tests to obtain droplet data by measurement directly. A fairly inclusive list of variables and dimensionless groups having been proposed to correlate rainout data are then systematically compared against the reverse modelled data. Acceptable correlations were claimed for droplet size in terms of superheat, partial expansion energy, extended flash fraction and bubble growth rate. Poor correlators of data were concluded to be the Jakob number, flash fraction and expansion energy. However, this exercise is further limited by the fact that data is compared against the particular thermodynamic variable, whilst other influential variables such as drive pressure and orifice size are also not constant across the series. A brief discussion is presented with regard to the influence of overpressure on the data, and a suggested modification of one of the dimensionless groups to accommodate this, but this is not considered sufficient. The data should be represented and grouped according to conditions where one variable is changed at a time, with the others remaining constant.

AEA review of CCPS book

Ramsdale and Tickle[9] go some way towards addressing some of these issues, deriving some useful general conclusions. They emphasise again the difficulties facing Johnson and Woodward due to the lack of source droplet size data or an appropriate correlation. In light of the difficulties RELEASE has in reproducing the observed rainout efficiencies from CCPS programme - not least because of the omission of evaporation processes - the authors suggest that at this stage of development, it may be more appropriate to use direct correlations – advocating the method of De Vaull and King[67] – to predict rainout. They represent the De Vaull and King correlation against some of the CCPS data to show reasonable performance, but indicate that it is not known how this correlation will perform for conditions outside the range tested via the CCPS programme. The adoption of such a correlation as a short term measure does seem at least as good as any other method that can be proposed at present, so long as this is coupled with a strategy to replace it with a physically based model in the medium-term in the interests of generality.

Here it is proposed that a mixed strategy be adopted whereby the usage of a simple correlation may be adopted as an appropriate option for the short term, whilst more general correlations are being developed to facilitate improvements of more physically based models. The simple correlation of De Vaull and King for volatile releases is represented as :

$$\eta_R = \eta^*_R \left(1 - \{x/ 0.145\}^{1.8}\right)$$

provided $x < 0.145$ and $\eta_R = 0$ otherwise. In the above correlation,

$$\eta^*_R = 1 - 2.33\{(T_a - T_{as})/T_a\}$$

and x is the isenthalpic flash fraction.

For non-volatile cases, the correlation recommended reduces to :

$$\eta_R = 1 - x - C_{pL} (T_{sat} - T_{as})/L$$

The proposal by Kletz[68] is found to perform not so well :

$$\eta_R = 1 - 2x$$

Ramsdale and Tickle[9] also derive some useful trends of general note. They emphasise the potential influence of variation of droplet size distributions and the difficulties with regard to rainout efficiencies in representing distributions as a single mean quantity. They also segregate the CCPS data to a certain degree – as advocated earlier in this report– to show the dependence of rainout on the primary control variables. They conclude that in addition to the dependence upon superheat, rainout is more sensitive to drive pressure than orifice size. Note that these trends are consistent with the new correlation proposed for mechanical break-up herein. A further development of this useful approach would be to attempt to segregate the data into flashing and non-flashing cases, and then to compare the sensitivity of rainout to the three primary variables for the flashing and non-flashing groups independently. The approaches adopted by Muladidhar[18], Ramsdale and Tickle[9] proposed in this report are all consistent in that the influence of control variables (or of course appropriate non-dimensionalised representations) are considered on an independent basis before data reduction is attempted. It is strongly recommended that the basis laid out in these three reports be continued in future investigations to allow model development and ease of use of data between experimental programmes from different sources.

EEC programme STEP

The data generated as part of the STEP programme[14], subject to the intrusive method of obtaining valid measurements and the transient characteristic of release conditions (which was noted not to have induced a temporal variation in the diagnostics measured), nevertheless represents a very important benchmark for the source term for flashing jets. The contaminant and the chosen release conditions for the primary variables are representative of a truly flashing jet, and so it is advocated that future models proposed for flashing jets should be tested against the data points from this programme.

The fluid utilised is high purity (99.5%) liquid propane, released into atmospheric conditions. The release conditions varied were exit orifice diameter (2,5, and 8mm) and initial storage pressure (5, 11, 17bar). The propane is stored under saturated conditions, so superheat would have varied as a function of storage pressure. Measurements were undertaken at 3 downstream axial locations, utilising a PDA system as discussed earlier. It was found that whilst a decrease in droplet size was noted along the axis of the jet – due to evaporation – even closest to the nozzle, no droplets greater than 80μm were recorded. Clearly this is markedly different from Mechanical break-up conditions (Figure 10), and any modelling approach advocating mechanical break-up for these conditions must be in error. The effects of evaporation were also clearly noticeable in one set of radial droplet size measurements, as mean sizes decreased towards the edge of the jet. For 5 bar releases at 60mm downstream, the measured SMD varied between 39-49 μm for the 2mm and 5mm cases respectively. At 11 bar at 60mm downstream, the droplet sizes reduced to 30-31 μm for the two orifice sizes. These measurements indicate the very small influence of orifice size at the higher pressure, and the more significant dependence of droplet sizes on release pressure and superheat (these two effects cannot be decoupled from

this series). At 17bar, SMD droplet size was below 30μm at all locations for the 2mm and 5mm orifices.

Regarding implications for rainout, these results indicate that very little if any rainout would be expected from a 11 bar release based on the sizes of droplets alone, whereas for the 5 bar release, evaporation would have to be modelled to assess the likelihood of rainout. The anecdotal evidence of little rainout from LPG releases seems consistent with this dataset.

Some other notes of general interest to add to the phenomenological interpretation of flashing jets, are that in all cases the characteristic bell-shaped jet was observed (Figure 7). This does seem a universal characteristic of flashing jets. Moreover, the diameter of this jet increased significantly with storage pressure (pressure and superheat). The velocity distributions appear to follow the Gaussian trends noted in other studies (though self-similarity has not been appraised), whilst the droplet size distributions also seem to be well-behaved, and would readily lend themselves to traditional generalised equations such as the log-normal or Rosin-Rammler as source information for a dispersion model. In general the range of droplet sizes is rather narrow. Finally, it is worth noting that the programme included data regarding void fractions at the orifice exit, which will prove extremely useful as improved models of flash atomisation based on two-phase flow within the exit pipe develop.

The corresponding modelling programme, proves to be rather disappointing from an atomisation perspective. An earlier correlation is quoted for the maximum droplet size within the spray, which under the conditions of the release, predicts 10μm. Whilst this is an order of magnitude less than that observed in the experiments, the authors continue to use this prediction in their future calculations[vii], claiming this to be near the measured maximum droplet size, whereas the difference is likely to have a very significant effect. Hence, the claimed agreement must be subject to question given the inherent errors adopted in the initial input data, and consequently it proves difficult to comment on the appropriateness of the proposed strategy for modelling two-phase jets.

HSL experiments by Allen

The series of papers published by Allen[35,40,41] represent several years experimental study undertaken by the UK Health and Safety Laboratories as part of a CEC joint-industry project on a rig specifically developed for characterisation of two-phase flashing releases. Again LPG is considered as the test fluid, and the work represents progress towards providing a reliable benchmark data-set against which source term models can be verified, and the appropriateness of different characterisation methodologies for flashing release characterisation – see section 3. The release conditions are reported to have mean release temperature of 16 °C and mean mass release rate of 0.0951 kg/s at saturated conditions. The nozzles utilised in the published work were of 4mm exit orifice size with L/d =10. The researchers commendably persevere to avoid intrusive measurements in the harsh operating conditions provided by flashing releases, and hence attempt to improve upon one potential error source in the STEP[14] programme. This invariably means that non-standard hardware and operating procedures have to be adopted and the data post-processed considerably.

Consistent with the recommendations of this report, LDA measurements provide sufficient particle velocity component quantification after data post-processing, and LIF is developed towards quantification of jet temperature – this could be developed towards providing relative phase information also. However, the choice of particle size diagnostic technique is not considered the most appropriate due to the problems of laser obscuration and vignetting discussed in section 3, although the authors endeavour to process the data towards quantitative

[vii]It is not clear from the STEP paper why this simplifying assumption was adopted.

size information. The data before manipulation shows 3 characteristic particle size peaks. After data manipulation, useful size information is provided subject to the appropriateness of the manipulation process, and the data is reduced to a bimodal distribution, where the majority of data is noted to be less than 32 μm. Data is subsequently presented in relative size bands – normalised against the total spray volume - where repeatability of the analysis technique is demonstrated. The authors recommend that the data at any point should not be considered in absolute terms, but rather in terms of identifying general trends and overall size distribution behaviour. In this sense, for trend analysis compared with other data-sets and models, the indication that the majority of the data is 30 μm or less means, as a broad estimate accounting for the disproportionate influence of larger droplets, SMD values of the order of 30 μm would be appropriate.

The approach adopted by the HSL group to post-process the diffraction-based data is considered plausible ; it is very doubtful that any better could be achieved using the diffraction technology. Hence, this programme serves the purpose of providing qualitative benchmarks, whilst emphasising the inherent unsuitability of diffraction technology for the environment of flashing sprays.

AEA review on droplet formation and rainout from two-phase releases

The current review was initially carried out independently from another AEA review on droplet formation and rainout from two-phase releases[69]. Hence the generally similar general philosophy and conclusions for many of the aspects is encouraging. None of the primary conclusions of this work changed as a result of the AEA review, though some additional equations were added for comparative appraisals. The authors concur that the adoption of transition break-up criteria is more favourable than a minimum value from two independent processes previously utilised. An additional criteria previously proposed governing flash jet break-up is proposed, which should be compared against the Kitamura correlation [49] suggested earlier. Reference is made to the work of Tilton and Farley[70] - developed from the earlier work of Lienard and Day[51] - who proposed a series of correlations of direct relevance to this study. Tilton and Farley suggest droplet size correlations for the capillary regime (which will not be of relevance to atmospheric dispersion problems), aerodynamic (mechanical) break-up regime and the flashing regime. The latter two regimes are represented by:

$$d_p = 0.585.u_0^{-1}.(\sigma/\rho_L)^{0.5}$$

and

$$d_p = 5.10^{-4}.(2\sigma/\rho_g u_0^2)$$

The mechanical break-up correlation is independent of orifice size, but the exponent for the exit velocity is within the range of values previously measured. A small sample of calculations using this formula indicate plausible droplet size estimates, and a fuller comparison should be considered. The flash correlation is relatively independent of degree of superheat – apart from the relatively small influence of temperature on liquid properties – and appears to predict excessively small droplets, hence possibly being over-conservative, though this again needs a fuller appraisal. However, the approach of utilising a transition criterion coupled with generalised independent droplet size correlations is fully consistent with that advocated in this study. Further reference is made to studies from the nuclear industry, and in particular the work of Koestel et al.[71] appears to be very useful, in that a correlation is provided based on the two-phase flow upon release. This type of approach has already been advocated in this review for future models of flash atomisation. Clearly an appraisal of the model of Koestel et al. against the experimental data available is in order. Finally, the authors present a concise summary of the

relevant large-scale release data in this area, in addition to the CCPS programme[7]. Of particular note are the data-sets where no rainout was measured, which are obvious candidates for validation studies.[viii] The overall methodology proposed for predicting atomisation from flashing jets at this stage of development is fully endorsed, and the fact that the authors differentiate between internal and external flashing is also very encouraging. The approach proposed for rainout and cut-off is rather less clear in that 'reverse modelling' is advocated, but perhaps this is the only option for users at this stage of development.

4.3.5 Flash atomisation of binary and multi-component fuels

Clearly without a consensus on appropriate models for single-component flash atomisation, it may be considered rather premature to consider multi-component fuels. However, in real-case scenarios users of dispersion codes will have to make some decision on how to 'simplify' multi-component fuels to provide suitable input parameters to the model. Very few published studies have considered multi-component fuels, the few studies that have been undertaken concern the practical application of deodorant aerosols. For the deodorant application, a propellant with vapour pressure below the anti-bacterial component is used in a pressurised container under conditions conducive to flash atomisation being realised when released. Again reference to Figure 2 elucidates the phenomenon.

Sher and co-workers appear to be the main group of investigators in this area over the last 30 years. The first paper in this series[37] proposed a new model for flash atomisation from aerosol canisters based on nucleation and bubble growth rate. Flashing is assumed to occur when the bubbles touch – a geometric criterion – after which the bubbles explode so producing the aerosol. On the basis of this assumed phenomenology, an equation is produced to represent d_{50}, the number median diameter, as a function of thermo-fluid properties of the binary system and some parameters of the model process. Interestingly, the model predicts independence of orifice exit diameter – which is consistent with effervescent atomisation – a corollary which is verified via an experimental test programme undertaken. However, the authors point out that this may not be universally true for flashing jets, as the data of Brown and York[48] did show a dependence of particle size on orifice diameter. The reason for this discrepancy is proposed to be due to the place where nucleation takes place i.e. for internal flashing spray quality is independent of exit orifice, whereas for external flashing there is a dependence.

More recent papers[72] consider the implications of binary fuel mixtures. Mixtures of ethanol as the dispersant and Freon-22 as the propellant were used for convenience. Initial conditions ranged between 2-8 bar for drive pressure, 25-60 C initial fluid temperature and with orifice size around 1mm. An expansion chamber is included along the discharge line, which it is claimed has been established as an empirical method for controlling spray characteristics for over a century. The important conclusions are that the spray quality is not affected significantly by the characteristics of the expansion chamber, save for an intermittent spray persisting for very short chamber lengths. Data was provided using diffraction-based droplet sizing technology, and the data for various mixtures of propellant/dispersant were found to collapse onto a single curve if plotted against a modified Jakob number, whereby the molar fraction of the propellant in the pressurised container is used as a pre-multiplier i.e. :

$$Ja^* = x_\beta \, C_{pL} \, \Delta T_{sh} / h_{fg}$$

[viii] None of the 2-phase experiments in the SMEDIS and Hanna's datasets of experiments resulted in any substantial rainout. In agreement with this, none of the UDM[1,2] simulations of these experiments resulting in any substantial rainout. Note however that in case of no rainout, the simple HEM thermodynamics formulation (not solving any droplet equations etc.) results in very close predictions to that of the sophisticated non-equilibrium droplet thermodynamics formulation. As a result experiments with a substantial amount of rainout are required, for a more complete validation of the UDM droplet modelling.

The measured SMD values range from 10-70μm, showing a considerable dependency upon drive pressure differential, and internal orifice characteristics (shape factors). Evidently once understanding of the influence of primary flash atomisation variables has developed, then the influence of orifice dimensions has to be considered to develop modelling approaches further.

A Sauter Mean Diameter correlation is proposed between initial conditions of the primary solution and the spray quality for a binary mixture[73] :

$$d_{32} = ((1-\eta_{\beta,st})/\eta_{\beta,st})\ 6\sigma/\{\ \eta_n \rho_\alpha R_\beta T_a \ln [P_{sat}(T_{st})/P_a]\}$$

The generality of this correlation is not known, and would have to be appraised relative to data of relevance to atmospheric dispersion problems.

It should be mentioned in this section that Muralidhar et al.[17] develop a model for predicting rainout from multi-compound mixtures including HF and additives. Although superheated, the releases are claimed to have been dominated by mechanical break-up processes. As such, a variation of the Weber number approach is adopted, and no rigorous treatment of the multi-component nature of the atomisation process appears to have been included. This was not considered further given the complex thermodynamics involving HF polymerisation.

Studies of binary mixtures are few, and no papers concerning the atomisation aspects of flashing releases of multi-component mixtures have been identified. At the lowest level, it would seem intuitive that atomisation would be controlled by the component with the highest vapour pressure, though clearly this is an area where considerable research is required.

4.4 SUMMARY

The hazard generated by accidental release of volatile liquids is generally considered to be the quantity of airborne matter. Hence, the magnitude of the hazard is inversely related to the quality of the spray – essentially, the characteristic size of droplets generated.

Most current jet dispersion codes divide the process of atomisation of superheated jets into two possible outcomes governed by different mechanisms: The first is termed ‘mechanical break-up’, the second ‘flashing break-up’. The mechanical break-up mechanism is considered to be independent of the thermodynamic state of the jet, whereas for flash atomisation, thermodynamics dominates. This level of differentiation is endorsed within this review, as there is a considerable body of evidence which shows that for low degrees of superheat there appears to be little qualitative difference between jet break-up under these conditions and for a sub-cooled jet release. This has not been proven on a quantitative basis, and this should be undertaken in future studies, but considering domination of mechanical break-up over a range of superheat is consistent with the current level of understanding.

There is inconsistency within the literature as to when either mode dominates for a particular problem. Most atmospheric dispersion models utilise methodologies for quantifying sprays generated from both mechanisms, and then take a minimum value of the two as a conservative estimate. This is considered unsatisfactory, and not defensible in light of existing information. All but one of the references reviewed indicate that when flash atomisation prevails, the sizes of the droplets so produced decreases. At the very least, this information should be represented within the model. Some dispersion models of flashing jets refer to mechanical break-up being the dominant mode, which is clearly inappropriate. There has been some work undertaken which attempts to define a transition criterion governing which mode dominates. Although only

partially validated, in the absence of any other information, it is proposed that this approach should be appraised against the experimental data available, and adopted as an improvement on current practice in dispersion codes whilst exploratory studies concerning a transition criterion are sought.

Concerning the methodology for deriving spray characteristics for the different modes, for mechanical break-up all dispersion codes currently utilise the critical Weber number criterion derived from single droplet studies. Critical Weber numbers – governing the relative role of momentum versus surface tension in droplet break-up - utilised vary between 10-22.

On a physical basis, numerous studies utilising a variety of appropriate laser diagnostic techniques have shown that pressurised releases of liquids in the form of jets break-up at first order according to the size of the orifice, the exit velocity of the jet (or pressure) and the fluid properties. Other parameters such as orifice characteristics are also known to be influential. The single droplet Weber number criterion does not represent this body of information, in that it is independent of orifice size, and its scaling with release velocity (or pressure) is inconsistent with the range published via empirical correlations. On this basis, the current methodology for characterising sizes of droplets in spray releases under mechanical break-up is considered inappropriate.

In the short-term, this methodology should be replaced with one of the correlations available in the literature, which provides an estimate of the appropriate mean droplet size for this type of heat and mass transfer problem, the Sauter Mean Diameter (SMD). A new correlation recently derived and validated for conditions more appropriate to hazard releases is advocated, which does represent the variation of pressure and orifice size consistently with recent data. This correlation does show that unobstructed releases of fuel through large orifices at low pressures can be assumed to scale from the earlier correlations derived for conditions more representative of diesel injectors. Whilst downstream processes will clearly play a role, the dependence of mechanical break-up atomisation on drive pressure and orifice size should be generally represented in rainout data from experimental studies, and there is some evidence of this consistency, though a full study of this has not been possible within the timescale.

The position regarding an appropriate methodology to quantify flash atomisation is far less clear. Current atmospheric dispersion models proposed either attempt some variation of the critical droplet number approach, or are based on correlations derived from ‘reverse’ modelling using a dispersion code to derive initial droplet sizes. Neither approach is endorsed here as a suitable method for quantifying characteristics of the spray. However, the latter is considered a useful exercise in an attempt to identify trends. Of course the ideal would be to measure the sizes at source whilst measuring rainout, but this has proved an extremely difficult proposition at any reasonable sort of scale. The ‘reverse’ modelling approach of course relies on all the other aspects of the dispersion model being sufficiently accurate, but in light of the review in the following section, prioritising the deficiencies in current methodologies, this seems a reasonable assumption.

This review has revealed that beyond the superheat limit for mechanical break-up, there are several modes characteristic of what is generically termed flash atomisation, the distinction being where vapour production first commences – upstream or downstream of the exit orifice. No simple methodology for predicting transition between these different modes has been found. Models have been developed that consider downstream bubble production, and it is seems plausible that these types of models could be adapted for the jet dispersion problem, but this is a longer term proposition. For the case of vapour production upstream of the orifice, it is proposed that the downstream atomisation should be correlated to the flow characteristics and dynamics at the exit orifice – at the very least the void fraction at the exit, and ideally the distribution of the phases (annular, slug, bubbly, etc..). There is a significant body of work

including modelling from the heat transfer literature that develops downstream characteristics of flow from upstream boundary conditions. This type of approach is considered potentially useful for longer-term development of a more robust approach to modelling flash atomisation.

The recommendation in the short term for quantifying the flash atomisation process is that at the very least the characteristic size of droplets under flash atomisation conditions should be less than sizes predicted by mechanical break-up. Moreover, there is a very strong analogy between flash atomisation and a technique (effervescent atomisation) that has been developed over the past ten years to mimic flash atomisation by producing two-phase flow within injectors similar to that characteristic of fully flashing conditions. This report has revealed that most of the qualitative descriptions reported for flashing sprays are fully consistent with published work on effervescent sprays. There is considerable potential for model development and validation if this consistency could be extended to justify quantitative equivalence. The particular properties that have shown commonality – albeit compared with the limited data available for flashing jets – include : independence of orifice size, dependency on drive pressure, uniformity of mean spray sizes across transverse sections, Gaussian transverse velocity profiles and self-similarity of these velocity profiles in the axial direction.

At a qualitative level, ironically, the modified critical Weber number approach does show both an independence of orifice diameter and inverse dependence on drive pressure. This is likely to be coincidental. The reverse modelling approach, aside from its weakness in terms of scientific rigor already mentioned, is further hindered by the fact that data is presented where both dynamic and thermodynamic parameters are varying. Hence, it is not possible to immediately determine whether indicated droplet size correlates well with a thermodynamic parameter, as the pressure effects, possible orifice size effects, and fuel property effects will also have influenced the data.

The most consistent conclusion derived from this review regarding flashing sprays is the intuitive one that mean droplet size and superheat are inversely related. The actual form of the correlation between these two variables, is not consistently reported. Hence, at this stage of development and consistent with general risk and hazard modelling practice, one has to err on the side of conservatism guided by the very few data-sets presenting droplet sizes for medium-scaled flashing releases. Hence, if a jet is predicted to atomise by the flashing mode under relatively high superheat (> 40 °C), then an estimate of 30μm for initial SMD is recommended based on the liquefied propane release PDA data from the STEP programme[14], and the HSE flashing LPG data using the laser-diffraction methodology[40]. Under conditions of relatively low superheat (< 40 °C), an initial jet SMD estimate of 70μm is proposed[ix], which is larger than the fully flashing jet but smaller than the sizes predicted for mechanical break-up. One could adopt the effervescent analogy and hence include the pressure/orifice-size effects known for effervescent atomisers, proposing independence of orifice size, and an appropriate modification for pressure effects, but this is considered premature and more suitable as an appraisal programme for medium-term work. Again the influence of fluid properties could be adopted from the effervescent analogy, but with the same proviso applied.

In addition to mean droplet size, the spread or distribution of droplets produced in a spray will influence downstream rainout. Two established functions have been recommended in various papers to represent sprays from flashing releases, namely the Rosin-Rammler and log-normal distribution. Either is recommended for use in the current application at this stage, as errors from misrepresentation of distributions are of considerable lower priority compared with the influence of the mean droplet size. Certainly once confidence has been developed in a methodology for predicting mean droplet sizes, then more emphasise should be placed on

[ix] For practical use in consequence modelling a continuous specific formula for SMD should be provided (e.g. no discontinuity at 40C).

optimal representation of the size distribution, but at this stage of development, the current approach – using a log-normal representation - adopted in most atmospheric dispersion codes is considered reasonable. It should be emphasised that these comments concern the post-flash droplet size distribution only, and it is not obvious that this size distribution should remain self-similar as the cloud disperses downstream.

5. EXTERNAL EXPANSION TO AMBIENT PRESSURE

The various thermofluid processes which have been considered for this part of the problem are reviewed and analysed in a systematic manner in two EU-funded reports, published by Britter[4,74]. A more out-of-date review of expansion formulations is given by Van den Akker[3].

One-dimensional expansion models appear to adopt plausible assumptions from the onset, and apply conservation laws subject to the inherent 1-dimensional approximation. The flashing or depressurisation zone for under-expanded single-phase jets is defined to occur over a short downstream distance. During this phase of the jet, no entrainment is assumed. The transition plane between the entraining and non-entraining region is defined to be plane at which the final jet pressure equates to the ambient pressure (atmospheric for the types of problems specified here). This may be represented schematically as a control volume problem as shown in Figure 1a.

5.1 GOVERNING CONSERVATION EQUATIONS

The expansion model calculates the final conditions at the end of the expansion from the initial conditions. The final conditions are given by the unknown post-expansion data: area A_f, velocity u_f, temperature T_f or liquid fraction f_{Lf}, specific volume ν_f (= 1 / density = $1/\rho_f$), and specific enthalpy h_f

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 an unambiguous system of equations :

$$m_f = m_0 \qquad (5)$$

$$m_f u_f = m_o u_o + (P_0 - P_f)\, A_o \qquad (6)$$

$$m_f \left[h_f + \frac{1}{2} u_f{}^2 \right] = m_o \left[h_o + \frac{1}{2} u_o{}^2 \right] \qquad (7)$$

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 (m^2) 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.

The post-expansion data can subsequently be determined as follows:

a) Set post-expansion mass rate m_f from Equation (5)
b) Set post-expansion speed u_f from Equation (6)
c) Set post-expansion specific enthalpy h_f from Equation (7)
d) The post-expansion liquid fraction f_{Lf} can subsequently be set from the enthalpy equation $h_f = f_{Lf}\ h_L(P_a,T_b) + (1-f_{Lf})h_v(P_a,T_b)$, where h_L is the specific liquid vapour enthalpy and $h_v(P_a,T_b)$ the specific vapour enthalpy.
e) Set post-expansion density $\rho_f = \rho_f(P_a,T_b,f_{Lf})$
f) Set post-expansion jet area: $A_f = m_f/(u_f\rho_f)$.

The above formulation corresponds to that included in HGSYSTEM and PHAST[75], and also corresponds to the formulation recommended by Britter[4,74]. In PHAST the above vapour enthalpy, liquid enthalpy and density calculations are carried out rather 'exact' using a DIPPR material property database.

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 (5), (6), (7) may be referred to as the *exact* equations.

It is noted that application of the above equations (conservation of mass, momentum, energy) may lead to excessive post-expansion velocities for cases where turbulence becomes important (possible occurrence of supersonic speeds and shock waves). To avoid these excessive velocities, PHAST adopts a rather arbitrary cut-off velocity of the velocity. Ideally the formulation should be extended to include the effects of turbulence. Moreover the thermodynamic path may need to include non-equilibrium effects and/or slip. The authors are however not aware of a published and validated formulation, which takes these effects into account. As a result the above formulation is recommended (with a possible cut-off for post-expansion velocity), until an improved formulation becomes available.

5.2 ALTERNATIVE EXPANSION FORMULATIONS

Further approximations to the above 'exact' system have been proposed within various models proposed for the atmospheric expansion problem:

A. The isenthalpic formulation relies on the change in the kinetic energy being small (hence ignored) compared with the change in enthalpy, in which case the energy equation (7) reduces to conservation of enthalpy across the flashing zone (e.g. Fauske and Epstein[76]). Clearly a weakness exists if the change in kinetic energy across the flashing zone – which is known unambiguously from equation (6) - is significant.

B. The 'isentropic' formulation as referred to by Britter, replaces the energy equation (7) with an isentropic assumption, allowing use of the well-known isentropic thermofluid relationships. Thus it applies conservation of mass/momentum/entropy. This approach is adopted in the TNO Yellow Book (1979)[77], for example.

C. The 'isentropic' formulation as referred to as an additional option in PHAST, replaces the momentum equation (6) with the isentropic assumption. Thus it applies conservation of mass/entropy/energy.

Influence of simplifying the energy equation

It is straightforward to propose simple scenarios to exemplify the potential and extent of errors introduced by simplifying the exact system.

Britter[74] shows that for a single-phase gaseous release of 10 bar down to atmospheric pressure, the isenthalpic assumption leads to an error in the final temperature difference of 104K, compared to an error for the isentropic assumption of 42 K. Whilst simple calculations of this nature could be used to argue the case of using the isentropic assumption in favour of the isenthalpic, the point to be emphasised is that both will introduce errors, exacerbated at larger release pressures, and which will become more exaggerated in the case of a two-phase system.

For the more relevant case of a two-phase release, Britter chooses a relevant example from the so-called 'Canvey Island' test data, involving a release of pressurised LPG stored at 288 K. In this example, the isenthalpic assumption gave a post-flash vapour mass fraction of 0.33, whereas the isentropic assumption predicted a value of 0.29. The exact solution would vary depending upon release pressure of course, and taking typical release velocities of 50 m/s and 100 m/s respectively, predictions of 0.33 and 0.32 respectively are deduced. Clearly the isenthalpic assumption performs better in this particular example, but no generality can be inferred from this.

5.3 SUMMARY

For flashing jets which can be considered single-phase (liquid) at the orifice exit, the non-entraining control-volume approach resulting in equations (5), (6), and (7) are considered consistent with the spirit of the modelling approach adopted by programs such as PHAST and HGSYSTEM.

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 (5), (6), and (7)] be continued.

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 outline earlier, would provide the additional benefit of an improved model for the post-flash vapour mass fraction.

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.

The authors are not aware of a published and validation formulation, which include the effects of turbulence and/or non-equilibrium (slip). The latter effects may need to be taken into account in the case of large post-expansion velocities (supersonic speeds).

6. Two-phase dispersion downwind of expansion region

As indicated in the schematic of Figure 1b, beyond the non-entraining jet expansion region the jet begins entraining ambient air. The various processes contributing to the jet and droplet in this later phase are now discussed, each on an individual basis.

6.1 DROPLET EQUATIONS OF MOTION

The droplet kinematics are unambiguously defined thus :

$$\frac{dx_d}{dt} = u_{dx} \quad , \qquad \frac{dz_d}{dt} = u_{dz} \tag{8}$$

where the Cartesian co-ordinates (x_d, z_d) represent the horizontal and vertical components of the droplet position respectively, with corresponding velocity vector (u_{dx}, u_{dz}).

The horizontal component of droplet velocity is assumed to be equal to the overall jet velocity, so that there are no drag or body forces acting in the x direction.

Applying Newton's second law to the vertical droplet motion results in the equation:

$$\frac{d}{dt}[m_d\, u_{dz}] = F_{body} + F_{drag} \tag{9}$$

where m_d is the droplet mass. The body force represents gravitational effects :

$$F_{body} = (\rho_{cld} - \rho_{cL})\, g\, V_d \tag{10}$$

whilst the drag force is defined :

$$F_{drag} = \frac{1}{2} C_{Dd}(\mathrm{Re})\ \rho_{cld}\ A_d\ |u_z - u_{dz}|\ (u_z - u_{dz}) \tag{11}$$

In the above equations, ρ_{cld} is the overall cloud density, ρ_{cL} the liquid density, g the gravitational acceleration, V_d the droplet volume, A_d the droplet surface, u_z the vertical cloud speed, C_{Dd} the drag coefficient, and Re the Reynolds number.

The empirical equations representing the droplet drag function are presented in the UDM manual following Clift et al.[78] :

$$
\begin{aligned}
C_{Dd} &= 0.44 && \text{for } \mathrm{Re} > 985 \\
&= 24\ \frac{1 + 0.15\,\mathrm{Re}^{0.687}}{\mathrm{Re}} && \text{for } 2 < \mathrm{Re} < 985 \\
&= 24\ \frac{1 + 3\,(\mathrm{Re}/16) + [9\,\mathrm{Re}^{2}\,\log(2\,\mathrm{Re})]/160}{\mathrm{Re}} && \text{for } 0.1 < \mathrm{Re} < 2 \\
&= 24 / \mathrm{Re} && \text{for } 0 < \mathrm{Re} < 0.1
\end{aligned}
\qquad \textbf{(12)}
$$

where the Reynolds number is defined utilising the relative velocity between the droplet and the surrounding ambient medium. Similar equations are utilised in other atmospheric dispersion models[10].

Vandroux-Koenig and Berthoud[15] propose a simpler Reynolds number correlation based on the work for rigid spheres. Their recommendations for revised correlations are:

$$
\begin{aligned}
C_{Dd} &= 0.33 && \text{for } \mathrm{Re} > 508 \\
&= 13.87\ \mathrm{Re}^{-0.6} && \text{for } 1.916 < \mathrm{Re} < 508 \\
&= \frac{18}{\mathrm{Re}} && \text{for } \mathrm{Re} < 1.916
\end{aligned}
\qquad \textbf{(13)}
$$

The above correlation is inconsistent with the recommended correlation by Clift[78], and no justification was reported to replace Clift's correlation.

6.2 TURBULENCE AND ENTRAINMENT

As the jet moves downstream of the flashing zone, the turbulent characteristics of the jet promote mixing and entrainment of surrounding air. For a liquid jet such as LPG or ammonia, the effect of this dilution with air is to enhance evaporation and hence cool the entrained air, which can result in the formation of a binary or separate water aerosol component under its new saturated water pressure condition. Entrainment also slows the jet down, and hence has significant impact on the jet length.

Various models are utilised to model turbulence and its influence on mixing for process problems, probably the k-ε model being the most widely cited and one of the simplest of the differential equation form. For most phenomenological models, attempts are made to reduce the computational overhead still further by empirically modelling the required influence of turbulence, for the near jet dispersion zone, the entrainment rate.

Under these simplified conditions, the following system of equations is derived for a horizontal elevated jet[x]:

$$
\frac{d}{dx}\left[c\,u\,A\right] = 0 \qquad \textbf{(14)}
$$

[x] Note that these equations are oversimplified. In reality e.g. gravity forces should be included for a heavy plume in the right-hand side of the momentum equation (16); see e.g. the UDM model description[1] for more precise and complete equations, including e.g. heat and mass transfer from the surface.

$$\frac{d}{dx}\left[\varphi\, u\, A\right] \;=\; 2\,\pi\, R\, u_E \qquad \textbf{(15)}$$

$$\frac{d}{dx}\left[\varphi\, u^2\, A\right] \;=\; 0 \qquad \textbf{(16)}$$

where c is the contaminant concentration (kg/m^3), $\phi = \rho/\rho_a$ the normalised density (ration of jet density and ambient density), A the jet cross-sectional area, u its velocity and u_E is the entrainment velocity, which essentially models the primary effect of turbulence in this approach. The above equations represent conservation of contaminant mass, the air entrainment equation and the momentum equation.

The two most common equations utilised in atmospheric dispersion codes to model entrainment are the Morton-Taylor-Turner and Ricou-Spalding methodologies. Entrainment is strictly defined in terms of the component of surrounding air velocity which is perpendicular to the jet axis (u_E). The two correlations may be represented as :

$$\begin{aligned} u_E &= \alpha\, u \quad , \; \textit{Morton Taylor} - \textit{Turner} \\ u_E &= \alpha\, \phi^{1/2}\, u \quad , \; \textit{Ricou} - \textit{Spalding} \end{aligned} \qquad \textbf{(17)}$$

where α is an entrainment constant. It is known that ϕ tends to 1 at large distances downstream. See the paper by Webber and Kukkonen on two-phase jets[79] (and also Section 3.4.1 in the UDM theory manual[2]) for a detailed comparison of the above formulations and appropriate selection of values for α. Note that St. George and Buchlin[16] demonstrated by experiments that the Ricou-Spalding entrainment law is indeed valid for two-phase jets.

A more rigorous approach is offered by Vandroux-Koenig and Berthoud[15], who introduce turbulence terms into a system of 19 unknown variables inter-related via the conservation equations in an attempt to model flashing releases of LPG. The 10μm droplets presumed are considered not to disrupt or enhance the turbulence of the gas mixture by virtue of the low value of the droplet Stokes' number; they are simply expected to follow the flow induces by the eddy structures. A turbulent viscosity is required, which is modelling using the Prandtl mixing length model.

6.3 COALESCENCE

Various models are under development for coalescence, and some evidence exists for coalescence being more prevalent than usually anticipated in two-phase droplet models[80]. Sub-models for the coalescence process are likely to develop considerably over the next few years, but at this stage of development for the UDM droplet model, this is considered to have low priority until more substantial evidence of the role of coalescence becomes available.

6.4 HEAT AND MASS TRANSFER

All numerically-based gas-droplet models from the various industrial sectors rely on appropriate empirical relationships to provide quantification of heat and mass transfer processes between the phases. Moreover, again most of these correlations appear to be reasonably consistent.

The energy balance considering all modes of heat transfer between the droplets and the surrounding environment is :

$$m_d\, c_{pL}\, dT_d/dt \;=\; A_d\, h\, (T_d\text{-}T) \;+\; h_{fg}\, dm_d/dt \;+\; A_d\, \sigma\, \varepsilon\, (T_a^4 - T_d^4)$$

where the terms in the right-hand side represent heat terms as a result of conduction/convection, phase change, and radiation, respectively.

The conduction convection term is governed by a suitable Nusselt number - governing the relative conduction/convection contribution – correlation. This is usually expressed as a general dimensionless correlation of the form Nu = f(Re, Pr), which is derived from established experimental databases.

The phase change involves the rate of change of droplet mass due to evaporation, which follows the so-called 'd^2 law', and is quantified via another suitable non-dimensionalised correlation Sherwood number - which represents the ratio of the total mass transfer to the purely diffusive component - as Sh = f(Re, Sc). The Prandtl and Schmidt numbers are essentially non-dimensionalised numbers involving fluid properties, and vapour-phase properties are usually evaluated at appropriate mean temperatures. The radiative term is often ignored in engine modelling.

The Nusselt, Sherwood, Prandtl and Schmidt numbers are defined as hd/k, Kd/D_{ac}, $C_{pv}\mu/k$ and $\mu d/\rho$ respectively, where d is the droplet diameter (m), h the heat transfer coefficient ($W/m^2/K$), k the thermal vapour conductivity (W/m/K), K the mass transfer coefficient (m/s), D_{ac} diffusivity of the drop component into the surrounding medium (m^2/s), μ the dynamic vapour viscosity of material in air (kg/m/s), C_{pv} the specific heat of the vapour (J/kg/K), and ρ the density (kg/m^3).

Typical generalised forms of the Nusselt and Sherwood number correlations are :

$$Nu = c\,(a + Re^{\,1/2}\, Pr^{\,1/3})$$

Sherwood correlations commonly utilised include :

$$Sh = c.(a + b\, Re^{\,1/2}\, Sc^{\,1/3})$$

This approach is consistent across both engine and atmospheric dispersion models studied. Values of constants a, b and c for the Nusselt and Sherwood number correlations are evaluated via specific published experimental databases. This is undertaken in a systematic manner to derive appropriate values for the atmospheric dispersion problem.

6.5 RAINOUT

Rainout is simply defined at the mass of liquid effluent that is lost from the airborne mass due to droplet impact and immediate retention on the ground[xi]. Similar considerations are made in

[xi] Note that following rainout, part of the liquid may re-evaporate.

engine studies under the so-called process of impingement, but due to the decrease in appropriate length-scale by several orders of magnitude between the buoyancy-dominated atmospheric dispersion problem and the momentum-driven engine environment, little further useful comparison can be made. In atmospheric dispersion studies, the low settling velocities of typical clouds (hence low Weber and Ohnsorge numbers) mean that no secondary spray will result from droplets reaching the ground elevation. Rainout from impingement on surfaces in the near-jet field is not within the remit of this review, though has been discussed elsewhere recently[19,81].

As discussed in previous sections a distribution of droplet sizes results from a typical atomisation process, and hence their droplet spatial/time histories will differ, resulting in a wetted area which depends upon the magnitude of the statistical dispersion of the droplet population. For release conditions typical of atmospheric jet problems, atomisation via the mechanical break-up mechanisms will result in jets with narrow characteristic cone-angles, and large mean droplet sizes (100s μm). Hence, it is plausible that a considerable mass of liquid effluent will accumulate over a relatively small area of ground. Hence, the current practice in atmospheric dispersion modelling of simplifying the problem to that of a release of mono-disperse droplets landing, spreading and forming a pool from a single landing position, has some credibility in this situation.

By contrast, the characteristics of a release which undergoes flashing atomisation does not lend itself to such an approximate process. Cone angles tend to be much larger and droplet sizes considerably smaller than the non-flashing counterpart. Hence, subject to particular release conditions, a typical fully flashing release of a volatile substance is generally likely to give rise to a ground dew-like coating rather than pool, which could well evaporate very quickly for highly volatile liquids. This description would be true, for example, of a LPG or LNG release of several bar release pressure as considered in the STEP programme[14,15] or the HSL data of Allen and coworkers[35,40,41] It would appear that a full calculation (subject to the critical droplet size) rather than the point-source approximation is required at least for the flashing atomisation release mode.

A considerable body of work has been undertaken by The Finnish Meteorological Institute (Kukkonen, Vesala et al.[82,83,84] in collaboration with the University of Helsinki concerning the fate of freely falling single and binary droplets under varying initial conditions. The relevance to these studies in relation to the remit of the current work is now discussed.

Critical Drop Size Estimation

The computational overhead associated with a modelling approach can be reduced if a *critical droplet size* above which all droplets rainout can be estimated. For liquids with boiling point considerably below atmospheric temperature (e.g. LPG, LNG) atomising via the internal flashing mode, rainout seems unlikely under atmospheric conditions. More generally, everyday experience with typical aerosols would lead to the *intuitive* conclusion that droplets of the order of 20 μm[xii] or less for most realistic release scenarios will not rainout, but either evaporate before settling, or be carried along with the jet. This is consistent with experience of providing seeding for laser diagnostic studies, where particle sizes of 20μm or less are sought to ensure the particle adequately represent the gas-phase flow.

If these intuitive judgements could be substantiated, then a considerable saving in computational overheads for atmospheric models such as UDM could be exploited. The number-size droplet populations are grossly biased towards the smaller size droplets, whereas the majority of the

[xii]This is the opinion of the second author based on intuition and practical experience.

mass is contained in the upper region of the distribution – due to the cubic dependence of droplet mass on droplet diameter.

Several studies have considered this problem in some detail. In particular, Vesala et al. (1989)[84] proposed a detailed numerical model for the fate of freely falling droplets. This level of numerical analysis is considered inappropriate for a phenomenological model such as UDM[1]. However, the authors compared results from their model with a simplified analysis which provided an analytical solution to the problem. They compare critical droplet sizes for the full numerical solution with the explicit equation from the reduced analysis for releases of high volatility (ammonia) and low volatility (water) aerosols. The difference in model results is observed to vary with concentration and release height, and results show that the error between the two methods is smallest for the lower concentrations and release heights. It appears from the sample of results presented, that a height of 1m and 10 droplets/cm^3 (rather dilute) provide reasonable guidelines for upper limits of these parameters. Although the droplet concentrations are rather small, these initial conditions are not unreasonable in terms of a hypothetical starting position downstream of the release to ascertain whether rainout is likely or not. The critical droplet size for water under these conditions is calculated to be 47 μm and for ammonia 107 μm using the full numerical scheme. The simplified analytical equation derived by the authors is in error by 8% and 12% respectively. Both these values are consistent with the intuitive cut-off value of 20 μm suggested earlier.[xiii]

Now estimating the maximum droplet size to be approximately double the SMD, these figures indicate that for a water spray of SMD = 24 μm, and an ammonia spray of SMD = 54 μm, no rainout is expected from a height of 1m. Admittedly humidity and wind effects have not been included in these estimates, but certainly this rather simple methodology offers attractions to estimate cut limits for rainout. A spray with SMD of 26μm is difficult to achieve from any release at low drive pressure, and so it seems likely that under most practical situations the release of water will always provide some rainout. However, a flashing release is certainly capable of providing sprays with SMD = 60 μm or indeed considerably less, and so it is not surprising that sprays of volatile liquid are often quoted anecdotally to have provided very little or no rainout.

The simplified equation may be fairly easily derived, relying on a simple iterative scheme to solve a transcendental equation[82]. The final equation for the critical droplet size is:

$$r_M = [(9\mu\ B\ H/2\rho_L g)\ [1 - 0.204.Sc^{1/3}[\rho_L\rho_g g/18\mu^2]^{1/2[}[72\mu BH/\rho_L g]^{3/8}]^{-1}]^{1/4}$$

$$B = -\ 4\ M_v D_a C\ P/\rho_L R T_a\ \ln\ [(1-\ P_{sat}/P)/(1-P_a/P)]$$

If the lower cut-off limit for rainout is taken at 20 μm, then clearly the equivalent mass of vapour would have to be added to the jet. Furthermore, it would be sensible to conduct a sensitivity study of this proposal compared with full calculations, and compared against established data-sets to consolidate the simplification.

Calculation of the Stokes' number, which characterises the effectiveness of large-scale structures for moving droplets laterally in the mixing region, for typical release scenarios and 20 μm droplets indicates values of the order of 1. Again, this is consistent with the suggestion of a lower cut-off limit 20 μm.

[xiii] If droplets of 47um evaporate before hitting the ground, then 20 μm droplets certainly will. So the assumption is correct to not model the sub 20μm aerosol as droplets.

Wheatley[10] proposes an alternative approach in the HSE dispersion code TRAUMA, where rainout is determined by the trajectory of the largest droplet in the spray, as determined by the Weber number correlation, being outside the jet cone-angle - essentially empirically-based.

6.6 OVERVIEW OF FORMULATIONS FROM LITERATURE

The droplet formulation used by DNV's model UDM is consistent with the droplet equation of motion and heat and mass transfer equations given by Sections 6.1 and 6.4. A good overall comprehensive review of models and correlations has been described by Chapter 3 in the report by Ramsdale[69], and is therefore summarised here very brief only:

a) Wheatley's model TRAUMA[10] adopts a simple criterion for deciding whether droplet rainout-out occurs from a horizontal two-phase jet (either all liquid is removed or none). It consists of estimating the largest droplet-size downstream of the inlet, and then comparing the gravitational settling velocity of droplets of this size with the horizontal velocity of the jet. If this results in a trajectory close to the jet axis compared to the divergence angle of the jet, then rainout is ignored.

b) The option of 'Removal by wet and dry deposition' was added by Hanna, Chang and Zhang to HGSYSTEM (HGSYSTEM-MMES)[85]. It adopts a formula for the gravitational settling velocity of the droplets, which will cause the 'plume of droplets' to move away from the 'gaseous plume'. The droplet plume is assumed to have the same shape as the gas plume (but with a different tilt angle), and is assumed not to affect the gas plume. The particle size is user input, and not set from the release calculations.

c) Papadourakis[86] described the code MULTDIS. This model is based on similar droplet equations of motion as the UDM, but does not adopt equations for heat and mass transfer from the droplet.

d) Muralidhar et al.[18] generalised the UDM approach to allow for multi-compound releases including HF.

e) The DRIFT model[87] includes a model for taking into account the deposition of droplets from a heavy gas cloud, adopting an overall deposition velocity.

f) The Eulerian model MC3D developed by Vandroux-Koenig and Berthoud[15] (see Section 6.2 for description), and the rainout model by Kukkonen[83,84] (see Section 6.5 for description).

References from the automotive literature provide similar correlations to that utilised currently in UDM (VECTIS user manual, Liu and Reitz,[88]). Liu and Reitz[88] compare droplet trajectory data for droplets deforming and breaking up from a controlled experimental facility with predictions utilising the drag coefficients for spherical particles as employed in UDM. Due to droplet distortion effects occurring during droplet break-up, it was found that an accentuated effect of drag due to the non-spherical shape of the droplet had to be employed to improve agreement between data and predictions. A revised drag coefficient term is suggested under these conditions. However, as current atmospheric dispersion models utilise droplet drag effects after the droplet break-up processes have been completed, there does not appear to be the need to revise the equations currently employed in UDM.

6.7 SUMMARY

The UDM model in PHAST and its multi-compound generalisation by Murahalidhar et al. (Exxon-Mobil) seem to be the only similarity dispersion models, which include equations for modelling the droplet movement, droplet heat and droplet mass transfer processes. They are consistent with those employed in models from other industrial sectors, though the appropriateness of utilising the SMD as a single representative droplet on rainout requires reappraisal. Most other two-phase dispersion models assume more simplistic rainout calculations, such as use of gravitational settling velocities and/or an analytical rainout equations derived directly from the release conditions. No large-scale experiments with significant rainout have been identified, which would enable direct validation of these models.

Concerning the rainout criterion, the current practice of always modelling rainout as a spreading pool is rejected. Whilst there is some justification for this if atomisation is via mechanical break-up of the liquid jet, for a truly flashing jet this practice is not considered consistent with the phenomenon in hand. A far thinner film of liquid over a far larger area is envisaged, which will result in significantly more evaporation and mass transfer. Having to model droplet deposition in far more detail will inevitably result in a greater computational overhead, but this additional cost has been offset somewhat by the suggestion that 20μm should be considered as a lower cut-off limit for rainout. Some justification is provided to support this subjective proposition.

7. POOL SPREADING AND EVAPORATION

As summarised in Section 6, the basic premise of the flashing release scenarios considered in this report developing spreading pools due to rainout is considered unlikely to be appropriate. Considerable work on pool models was undertaken by the UK HSE in the 1980s. Webber[89] provides a very good summary of the development of models for pool spreading and re-evaporation from liquid spills and two-phase jet releases, the appropriate equations defining the system, and validation studies of the proposed methodology. See also Fannelop (1994)[90] for an overview of pool models.

Following rainout, the rate of volume change of liquid effluent on the ground is given by :

$$dV/dt = S - D - WA$$

where S is the liquid discharge rate, D is a drainage rate and W and A are the liquid surface regression rate (due to evaporation) and area of 'pool' respectively. Whilst S and D can be estimated providing boundary conditions of the problem, A and W have to be modelled in terms of pool spreading and vaporisation rate respectively.

A brief review of a number of available models is given below:

a) DNV's pool model PVAP is automatically invoked following rainout from a two-phase plume within the UDM dispersion model[1,2] (see Figure 1b). It carries out pool spreading/evaporation calculations, with the vapour from the pool added back to the original plume. The shape of the pool is assumed to be circular with uniform thickness. The pool may either boil or evaporate while simultaneously spreading, with different models used for spills on land and on water. Detailed mass and heat balances are kept, permitting variations in the temperature of the pool. For spills on water, solution of the spilled liquid is calculated, and also the reaction with water for ammonia. The model has been validated against experimental data. Potential further work includes (a) additional validation, (b) extension to multi-compound evaporation, (c) improved formulation of addition of vapour back to the UDM plume, (d) extension of UDM model to allow direct dispersion from a pool.

b) The HGSYSTEM model LPOOL is similar to PVAP. It assumes a triangular cross-section instead of a uniform thickness. It also allows for multi-compound releases, and includes the effects of containment in a dyke. However it does not allow for dissolution with water and reactions. LPOOL is linked within HGSYSTEM with the time-dependent dispersion model HEGADAS-T in order to model dispersion from a pool. HGSYSTEM does however not allow for modelling of rainout, and subsequent modelling of pool formation.

c) The AEA model GASP is described by Webber[91,92]. It involves a solution of two first-order differential equations (spread rate, force balance) instead of one as adopted by the above models. Unlike the above models, it provides an unified treatment for evaporation and boiling. The GASP model has been compared against the PVAP model by Webber; see the PVAP verification manual in the UDM Technical Reference Manual[2].

d) The UMIST model REACTPOOL[93] provides a similar methodology to PVAP regarding spreading law and heat balance. In addition it contains additional mass balance laws required for modelling reaction, and is linked with a UMIST cloud model (simple heavy-

gas-dispersion model) also allowing for reactions. It has recently been generalised from SO_3/oleum reactions (reaction with water to form H_2S0_4) to more general reactions.

Additional more advanced but more CPU-intensive methods are available (e.g. a shallow-layer pool model developed by CERC). Note that the above 'simple' models all assume circular pools. The UDM appears to be currently the only model which models the pool re-evaporation following rainout. Herewith it adopts the simplifying assumption that all rainout occurs at the same point (when the UDM droplet trajectory reaches the ground). In practice, rainout will not occur at one point but distributed rainout will occur and moreover for some cases pool formation will not even occur as already previously discussed in Sections 6.5 and 6.7. The latter processes are currently in investigation in a separated HSE-sponsored study by Griffiths et al.[94]

8. CONCLUSIONS AND RECOMMENDATIONS

The over-riding weakness of current atmospheric dispersion models for flashing jets concerns the quantification methodology used for atomisation. Until this deficiency has been addressed, then in particular validation of rainout predictions from dispersion models will not be viable. By contrast, models included within PHAST for the depressurisation region and downstream droplet heat and mass transfer processes in the entraining jet are generally scientifically reasonable, and consistent with those employed in models from other industrial sectors. However, the modelling strategy of adopting the SMD as the sole representation of the spray within these sub-models for rainout calculations coupled with the assumption of self-similar droplet distribution profiles downstream is likely to induce error, and needs reconsideration in further work.

Only two data-sets of near-field droplet characteristics from flashing releases are known to exist (HSL programme undertaken by Allen and EEC STEP project). Although these data sets may be useful for development and validation of expansion models (e.g. initial droplet size), they provide insufficient experimental data for calculations further downstream (droplet heat/mass transfer, rainout and re-evaporation). Therefore further experimental data will be required in the future for model validation. However priority should not be given to further large-scale experimentation until a more rigorous atomisation model has been developed, and full use has been made of the existing data in a systematic verification programme. Large-scale programmes should only be proposed in future on the basis of verification of mature models, i.e. after such models have been appraised systematically over a range of smaller scales.

The list of conclusions and recommendations deduced during the course of this study are listed below. Subdivisions have been introduced in accordance with the layout of the report.

Atomisation processes

1. There is sufficient evidence to support representation of the overall phenomenology of flashing jet atomisation as a sequence of atomisation processes, with transition between each process being governed by appropriate transition criteria. These criteria are likely to depend not only upon degree of superheat, but also flow conditions, fluid properties and the particular geometric characteristics of the release orifice. Methods of characterising transition criteria between various modes should be developed in longer term research programmes.

2. In the short-term, two processes should be adopted for superheated jets with one transition criterion distinguishing between them. The terminology 'mechanical break-up' should be used to represent the atomisation process when no bubble growth within the jet is evident, and 'flash break-up' is defined to represent conditions when bubble growth is important. Mechanical break-up dominates at lower degrees of superheat.

3. Two correlations have been identified which purport to represent transition between the primary mechanical and flash break-up regimes as defined above. The Kitamura[49] correlation is recommended at this stage simply on the basis that this is the more recent correlation, and developed in full knowledge and with reference to the work of Lienard and Day[51]. A comparative study of both correlations against all existing benchmark data should be undertaken immediately to determine which, if either, is most appropriate.

4. The influence of orifice characteristics (e.g. L/d_o, roughness, shape), fluid properties (e.g. viscosity, surface tension) and multi-component contaminants have not been investigated for any modes of atomisation for conditions relevant to the atmospheric dispersion problem i.e. relatively low pressure and large orifices. Some of these parameters (e.g. orifice $L//d_o$) are known to be very influential regarding atomisation quality, and require systematic quantification on a prioritisation basis.

Mechanical break-up process - recommendations requiring no further work

5. The mechanical break-up process should at this stage be considered similar to that for atomisation of sub-cooled jets through simple orifices, modified to account for the secondary effect of the immediate flash fraction. Characteristics of sprays generated via mechanical break-up are:

   i) Inverse dependence of mean droplet size on release velocity (or pressure);
   ii) Dependence of mean droplet size on final orifice diameter;
   iii) Dependence of mean droplet size on fluid properties such as viscosity, surface tension and density;
   iv) Dependence of mean droplet sizes on final orifice characteristics (e.g. L/d and roughness).

   Correlations (preferably in non-dimensional form) proposed to represent the mechanical break-up process should be consistent with these characteristics.

6. Many dispersion codes currently adopt the so-called critical Weber number criterion for mechanical break-up. This model was developed empirically from studies of break-up of isolated droplets in flowfields, but is considered unvalidated for direct application to the liquid jet problem. Moreover, the Weber number predicts atomisation quality to be independent of orifice size, and its dependence upon release velocity is inconsistent with all previous data and correlations. Hence, this approach is not advocated to model atomisation from mechanical break-up. The method of Tilton and Farley[70] is more reasonable in that it exhibits a plausible exponent of velocity within its correlation, although independence of orifice size is a less encouraging feature.

7. A recent comparison of a broad subset of correlations against a new data-set has resulted in a new correlation being proposed, which is appropriate for larger orifice sizes and lower pressures typical of atmospheric dispersion problems. Whilst there are still known deficiencies which must be corrected before application dispersion models (see recommendation 15), this correlation correctly predicts the characteristics 5i) and 5ii) specified in conclusion 5. This correlation is believed to be more representative of data currently available than that of Tilton and Farley[70].

8. The droplet size distributions from jets undergoing mechanical break-up may be represented by established distributions such as the log-normal or Rosin-Rammler. Useful simplified trends relating SMD and volume undersize for jets undergoing mechanical break-up are that negligible liquid mass is contained in droplets less than 10% of the SMD, and that over 99% of the mass is contained in droplets less than 180% of the SMD. These simple correlations may be useful in assessing rainout characteristics cheaply.

Flashing break-up process - recommendations requiring no further work

9. Consistently reported atomisation characteristics evident as a result of flash break-up are:

i) Inverse dependence of mean droplet size on degree of superheat;
ii) Inverse dependence of mean droplet size on exit velocity (or release pressure);
iii) Mean droplet size relatively independent of final exit orifice size (only limited evidence);
iv) Characteristic droplet size is significantly smaller than those produced by mechanical break-up process;
v) Reduced rainout;
vi) Self-similarity of the transverse axial velocity profile at different locations downstream from the exit orifice;
vii) Relative uniformity of mean droplet size across a transverse spray profile;
viii) Significantly increased cone angle of the spray compared with mechanical break-up under otherwise similar conditions;
ix) Dependence upon detailed orifice characteristics (e.g. L/d_0).

10. One method currently employed to quantify droplet size from flashing jets in dispersion models is the modified critical Weber number criterion. This is inversely dependent upon release pressure differential, and independent of exit orifice size. However, the flash model is not usually invoked, as mechanical break-up is usually predicted to dominate in practical applications. It is not clear on what basis a critical Weber number criterion would apply for flashing jets. UDM currently adopts the correlation recommended by Johnson and Woodward[7] based on partial expansion energy. Other correlations have been proposed for flash atomisation which should be systematically appraised in future studies, the most promising considered to be that proposed by Nagai et al.[65], where most of the primary variables of influence seem to have been considered.

11. As none of the flash atomisation correlations proposed are considered to be characterised sufficiently, a conservative 'intelligent system' approach based on known data and characteristics is proposed for predicting SMD from releases involving flash break-up in the short term. Acceptable data for SMD droplet size under flash break-up conditions for low pressure (< 20bar) releases range between the limits of 20 μm and 80 μm. Hence, when flash break-up is predicted for high degree of superheat (>40° C), an initial jet SMD of 30μm is proposed. When flash break-up under low degree of superheat (< 40° C) is predicted, an initial jet SMD of 70μm is proposed. This is broadly consistent with the large-scale droplet sizing data and large-scale rainout data, and reasonably consistent with other smaller-scale data based on water releases. Clearly this methodology is based on superheat only, with no dependence on other important variables such as release pressure and L/d_o ratio, which would have to be introduced as better correlations are developed from future experimental studies. A critical assessment of this proposed interim methodology against rainout data is required.

12. A relatively new design of atomiser – the effervescent atomiser – was originally developed to utilise the processes governing flashing jets to produce high quality sprays very efficiently. The characteristics of sprays from effervescent atomisers are fully consistent with all the flashing jet characteristics summarised in the previous conclusion 9, and also the quantitative data from the STEP[14] and HSL[40,41] flashing propane data. A large body of data exists with associated correlations which may well be directly related to the flashing jet phenomena, and this should be explored as a high priority. Air-to-liquid mass ratio is the dominant variable governing effervescent spray characteristics, which it is postulated here, may play an analogous role to the void fraction at the orifice exit for flashing jets.

13. The few droplet size distribution data presented for flashing jets indicate well behave functions that could be readily modelled by the standard functions such as the log-normal or Rosin-Rammler functions. Either may be used at this stage of model maturity.

Superheated jet atomisation - future work

14. To replace the short-term modelling approach for flash break-up atomisation, small-scale studies under controlled laboratory conditions should be undertaken to determine new correlations for transition criteria using appropriate dimensionless variables.

15. The new correlation proposed for mechanical break-up should be consolidated by developing it to include what are considered to be the most influential parameters currently ignored : The influence of orifice L/d_o and fluid properties, including confirmation of the weak influence of superheat on atomisation.

16. For jets atomisation via the flashing mode of atomisation, relationships between spray characteristics and the relevant fluid and thermodynamic variables should be derived, preferably in non-dimensionalised form, through controlled small-scale experiments. This should include analysis and generalisation of droplet size distribution parameters also.

17. Scaling laws for atomisation under flash break-up conditions will require development over reasonable, systematic ranges for release conditions.

18. A medium (controllable) scale data-set should be derived coupling near-orifice and downstream spray measurements with rain-out data. This data-set should then be appraised against PHAST predictions taking the PDA/LDA data as input to appraise the droplet dynamic sub-models of the code.

19. All future experimental studies of flashing jets should aim to include measurements of the void fraction at the exit orifice. Models have been previously developed to predict appropriate variables such as flow structure and vapour fraction at the orifice exit, from which downstream atomisation characteristics could be more suitably correlated.

20. For multi-component flashing releases, at this stage of development the release fluid should be suitably characterised to allow derivation of droplet size estimates using the same methodology proposed for single fluid releases. When applying the flash methodology, priority should be given to the most volatile component to accommodate the enhanced nucleation provided by more volatile components. For mechanical break-up, in the absence of any other guidance, averaging fluid properties is recommended.

21. Techniques recommended for future experimental studies of superheated jet atomisation are: PDA – droplet size; LDA – droplet velocity; LIF – relative phase quantification and jet temperature. All these techniques potentially offer spatial and temporal resolution. LIF will require some development, and all techniques will require some adaptation to counter the hostile conditions prevailing.

Jet Expansion

22. Simplification of the flashing jet phenomenon as a non-entraining flash region and entrainment region is endorsed.

23. The recommendations of Britter[4] are endorsed, in that the full conservation equations of mass, momentum and energy should be utilised as opposed to the isentropic or isenthalpic assumptions in the flash region.

24. The authors are not aware of a published and validation formulation for jet expansion, which include the effects of turbulence and/or non-equilibrium (slip). The latter effects may

need to be taken into account in the case of large post-expansion velocities (supersonic speeds).

Two-phase dispersion, rainout and pool formation

25. The UDM model in PHAST and its multi-compound generalisation by Murahalidhar et al. (Exxon-Mobil) seem to be the only similarity dispersion models, which include equations for modelling the droplet movement, droplet heat and droplet mass transfer processes. These sub-models are consistent with those employed in models from other industrial sectors, though the appropriateness of utilising the SMD as a single representative droplet on rainout requires reappraisal. Most other two-phase dispersion models assume more simplistic rainout calculations, such as use of gravitational settling velocities and/or an analytical rainout equations derived directly from the release conditions. There is some evidence that supports the use of some simplified models as cheap or interim methodologies for broadly assessing the rainout fraction, and this should be afforded some consideration.

26. Alternative approaches to the single droplet (SMD) approach for spray representation in the dispersion region require development. Some variation of the 'droplet parcel' ideology adopted in other two-phase industrial CFD applications should be considered in this respect.

27. In rainout calculations, it is plausible that a critical droplet size exists below which droplets will never touch down, and hence for a particular scenario may be omitted from the droplet calculations, with their equivalent mass represented as vapour. This suggestion should be appraised in a series of numerical test cases.

28. The CCPS data-set is of only limited value to appraise the new method of initial droplet-size calculation against rain-out data, since no direct measurement of the initial droplet size were made. Thus only experimental data of limited value exist for direct validation of rainout models. In the longer-term, it will be required to visit large-scale validation programmes, but with a view to verifying existing correlations developed at small scale, rather than using large-scale data to develop appropriate correlations.

    Ideally the first step towards validating the UDM code for superheated releases should be to compare a sub-cooled release of liquid using the new mechanical break-up correlation to check that the isothermal dynamic processes are performing satisfactorily. A sensitivity study could then be undertaken to investigate the effect of mean spray size and droplet distribution characteristics on rainout prediction. Water would be the obvious test fluid, with care taken over the influence of atmospheric humidity. Thus one can ensure that the dynamics of the system are well predicted. Subsequently the model could be further improved with regards the further complication represented by the thermodynamic aspects.

29. More computationally expensive CFD models exist for spray dispersion with turbulence modelling. The various simplifications adopted within dispersion models like PHAST could be appraised against more rigorous models for appropriate benchmark problems to complement or as a cost-effective alternative to experimentation

30. More rigorous atomisation and dispersion models for multi-component fuels will require development, but this should be undertaken when a good understanding of and methods for modelling the single component problem have been developed. The UDM could be generalised to multi-compound droplet dispersion using the method by Muralidhar et al.[18]. Prior to this, the UDM should however be extended using the two-phase, multi-compound, homogeneous equilibrium model, as currently implemented in HGSYSTEM.

31. The UDM model appears to be currently the only model allowing for automated calculations of pool formation following rainout, with vapour from the pool added back to the cloud. However it applies simplifying assumptions such as the rainout to occur at a single point (no distributed rainout) and the pool to be circular. This may be plausible if the mechanical break-up criterion is dominant. However in case of flashing atomisation, often a pool may not form, but instead a far thinner film of liquid over a far larger area.

NOMENCLATURE

A	cross-section area of jet (m^2)
A_p	area of pool on ground (m^2)
C	droplet number concentration (m^{-3})
c	contaminant concentration ($kg.m^{-3}$)
Ca	Bubble growth rate ($ms^{-0.5}$)
C_D	drag coefficient (-)
C_p	specific heat at constant pressure (J/kg.K)
D	binary diffusion coefficient
D_j	diameter of jet (m)
d	diameter (m)
d_p	droplet particle diameter (m)
d_{10}	number averaged mean droplet diameter for polydisperse spray (m)
d_{32}	Sauter mean droplet diameter – SMD – for polydisperse spray (m)
E	specific energy (Joules/kg)
F	force (Newtons)
g	gravity (ms^{-2})
F_p'	extended flash fraction (-)
f	liquid mass fraction (-)
H	release height (m)
h	specific enthalpy (J/kg)
h_{fg}	heat of vaporisation (Joules/kg)
Ja	Jakob number (-)
k	thermal conductivity (W/m.K)
L	axial length of nozzle from exit orifice to substantial upstream expansion, as indicated in Figure 1a (m)
M	molecular weight (kg)
m	mass flowrate (kg/s)
N	bubble nuclei density – number of bubble nuclei per unit volume (m^{-3})
Nu	Nusselt number (-)
P	pressure (N/m^2)
Pr	Prandtl number (-)
R	jet radius (m)
Re	Reynolds number (-)
r_M	radius of droplet for which drying time and gravitational settling time equate (m)
s	specific entropy (J/K/kg)
Sc	Schmidt number (-)
Sh	Sherwood number (-)
SMD	Sauter Mean Diameter (m)
S_p	volume rate of liquid deposition on ground (m^3s^{-1})
T	temperature (K)
ΔT_{sh}	degree of superheat (K)
u	velocity (m/s)
V	volume (m^3)
V_p	volume of pool on ground (m^3)
v	specific volume = $1/\rho$ (m^3/kg)

We	Weber number (-)
x	flash mass fraction (-)
(x,z)	horizontal and vertical spatial components (m)
y	mass fraction (-)

Greek letters

α	thermal diffusivity (m^2s^{-1})
ε	void fraction (-)
v	specific volume = $1/\rho$ (m^3/kg)
μ	dynamic viscosity (Pa.s)
η	mass fraction (-)
η_n	efficiency of particular injector (-)
η_R	rainout mass fraction (-)
ρ	density (kg/m3)
σ	surface tension (Nm^{-2}) (or Stefan-Boltzman constant for radiation)
Δ	difference

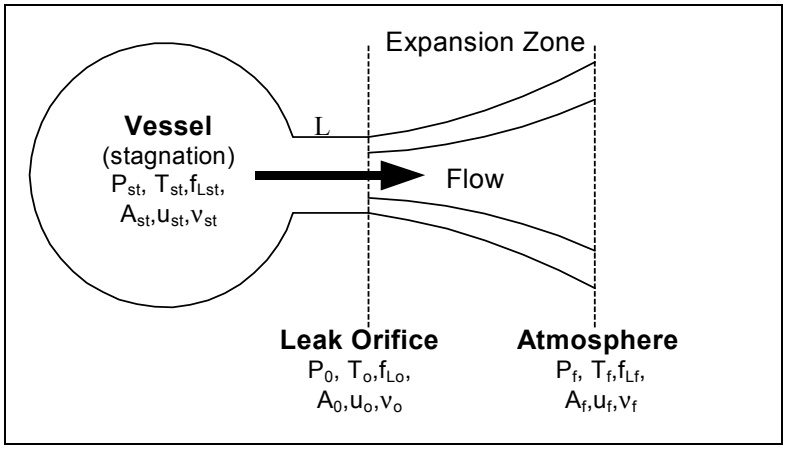
Subscripts

a	atmospheric
air	air
as	adiabatic saturation
b	boiling
body	body
cld	cloud
d	droplet
drag	drag
E	entrainment
f	final conditions after atmospheric expansion
G (or g)	gas
J	jet properties (liquid fluid properties used to non-dimensionalise variables)
L	liquid
l	initial conditions
o	initial conditions prior to atmospheric expansion (i.e. at leak orifice)
Re	Reynolds number
s	stream conditions
st	stagnation
sat	at saturated condition
sh	superheated
v	vapour
exp	expansion
p	partial expansion
x or z	x or z component
α	liquid to be dispersed
β	propellent

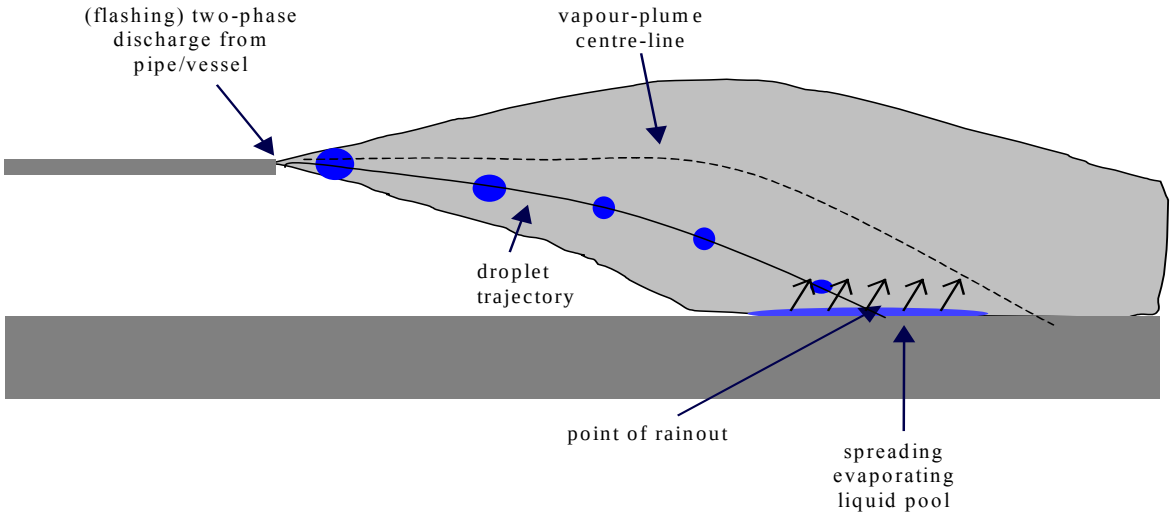
Superscripts

*	modified or non-dimensionalised

FIGURES



(a) discharge and atmospheric expansion



(b) two-phase dispersion (droplet movement/evaporation), rainout and re-evaporation

Figure 1. Phases in modelling: discharge to atmosphere, atmospheric expansion to ambient pressure, two-phase dispersion, rainout and re-evaporation

Figure 1(a) illustrates the atmospheric expansion to ambient following the release to the atmosphere. Release scenarios to be considered are:

(a) release directly from vessel or from pipe attached to vessel
(b) steady-state release (for small leak), time-dependent release (for larger leak) or instantaneous release (for catastrophic rupture)
(c) choked flow (exit pressure P_o larger than ambient) or unchoked flow (no expansion calculations needed)
(d) release of pure vapour, two-phase or pure liquid

Figure 1(b) illustrates the movement of the droplets in the downwind direction. If the cloud moves in the downwind direction cloud entrainment occurs and the droplets are evaporating. Since the droplet are more heavy than the surrounding vapour, the droplets typically move away from the cloud centre-line. Rainout of the droplets may result in the formation of a spreading evaporation liquid pool.

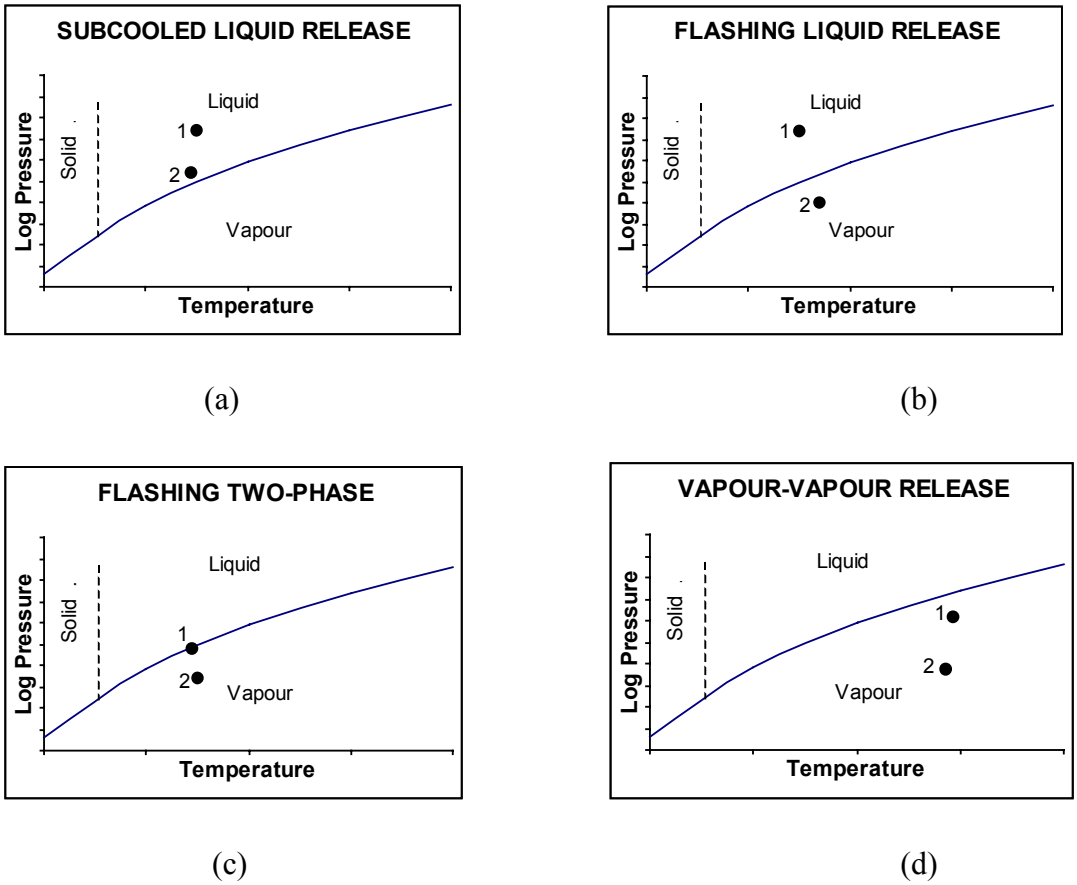


Figure 2. Thermodynamic boundary conditions in relation to saturated conditions

In the above figure:

- point '1' refers to the initial liquid stagnation conditions (pressure P_{st}, temperature T_{st})
- point '2' refers to the atmospheric conditions beyond exit (pressure P_a, temperature T_a).

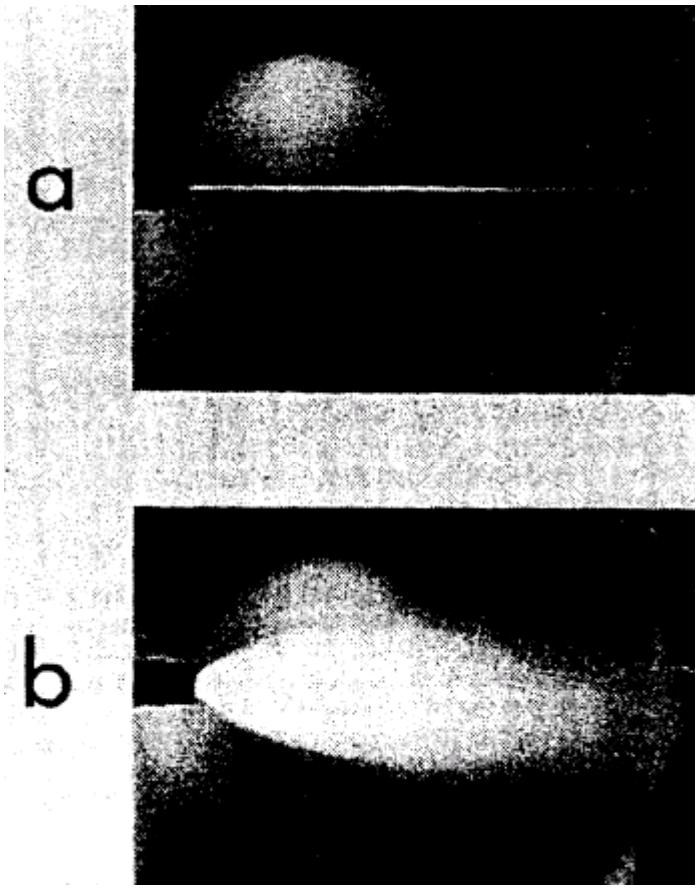


Figure 3. Visualisation of difference between non-flashing and flashing jets (Reitz)

Above photos of water jets are taken from Reitz[20]. The water jets are injected at (a) 300K and (b) 426K using scattered light illumination. The nozzle exit is at the left of each picture, and the flow is from left to right. The room temperature jet remains cylindrical (Figure a), while the heated jet (Figure b) diverges starting at the nozzle exit and appears to be well atomised.

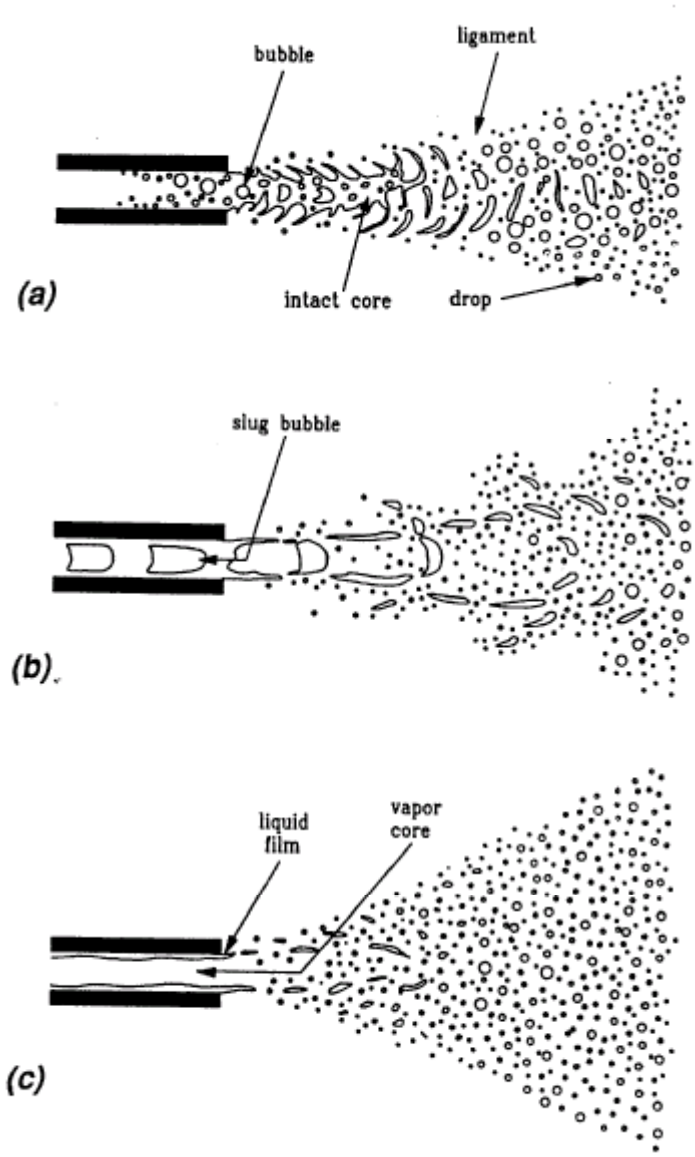


Figure 4. Dependence of spray characterisatics on upstream flow conditions (Park and Lee)

The above picture is based on interpretation of photographs and is taken from (Park and Lee, 1994)[21].

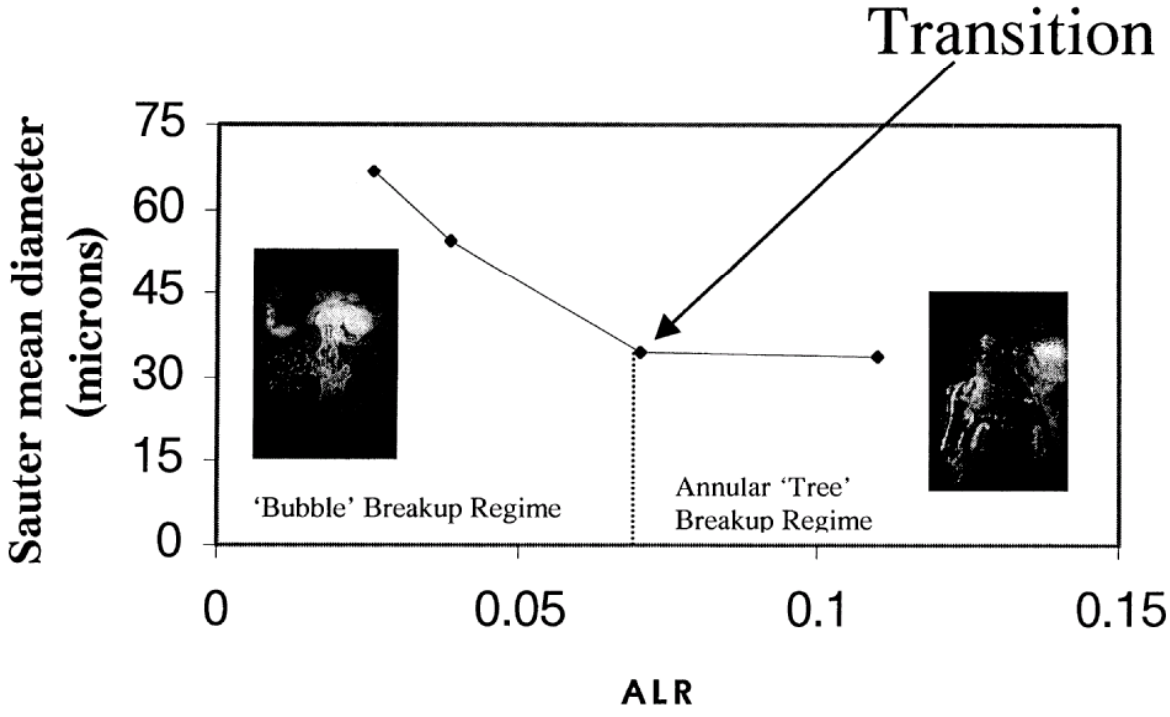


Figure 5. Effervescent analogy

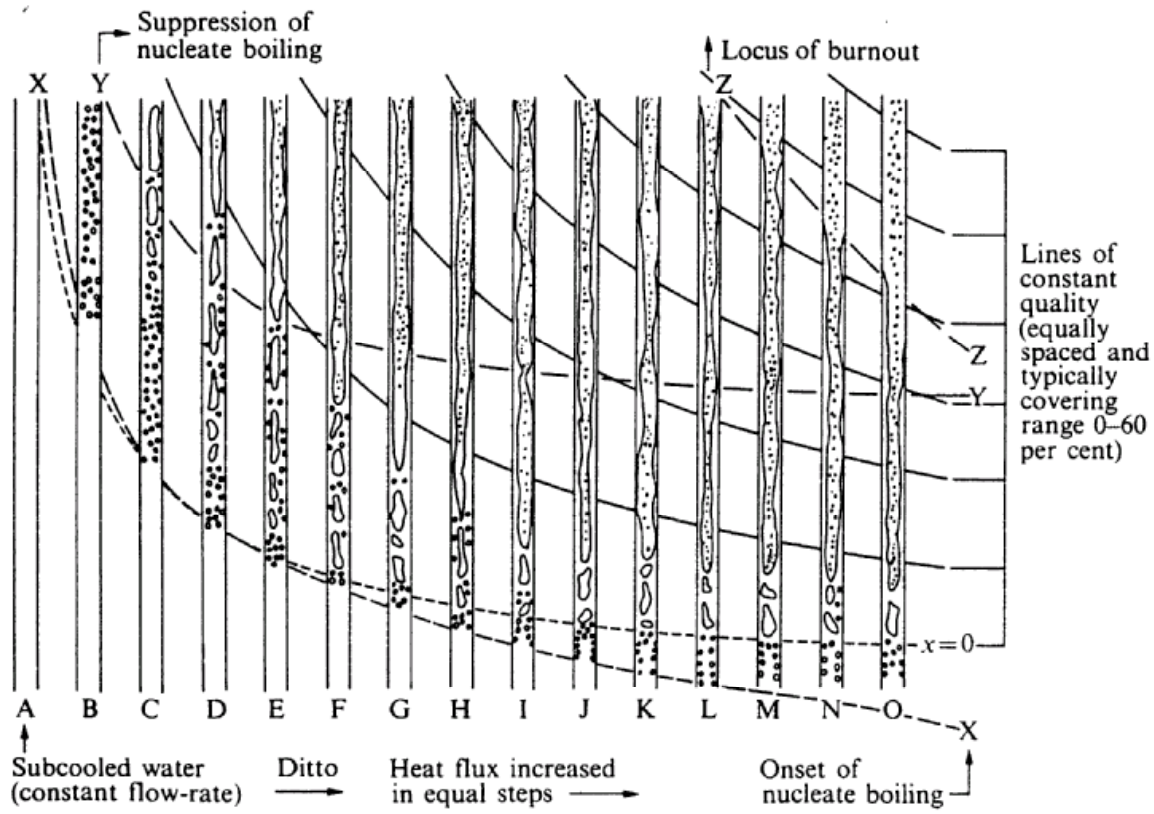


Figure 6. Schematic of variation of two-phase flow with increasing heat flux (Hewitt)[23]

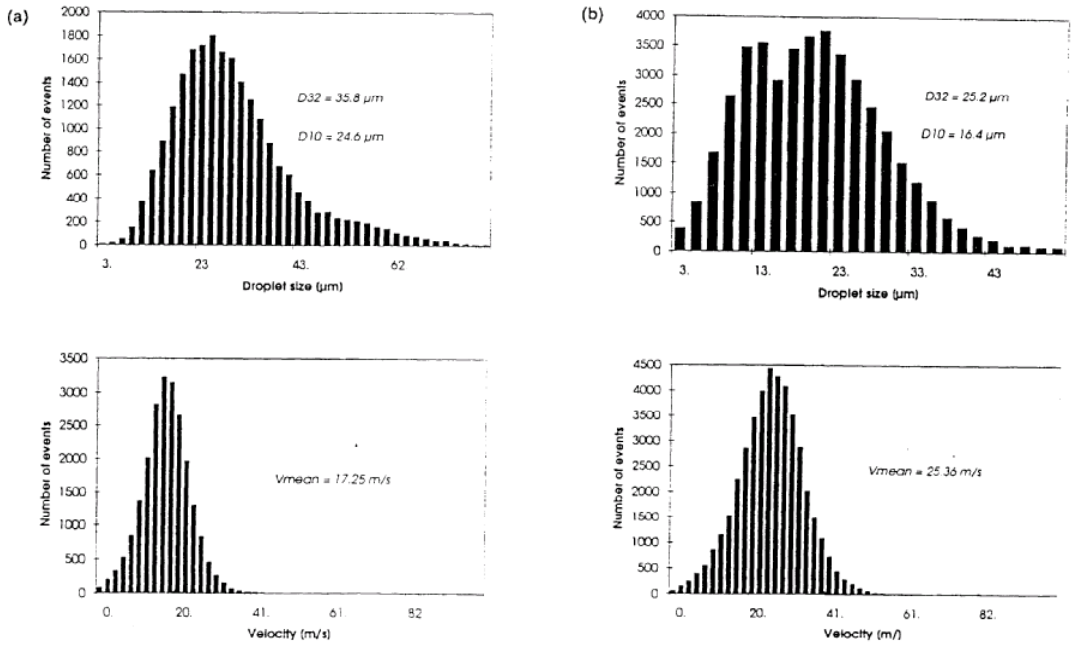


Figure 7. Droplet-size and velocity histograms for STEP PDA/LDA data

Results are given for release of liquid propane from 2 mm nozzle at downstream distance of 95 mm and with different initial pressures: (a) 5 bar (b) 11 bar

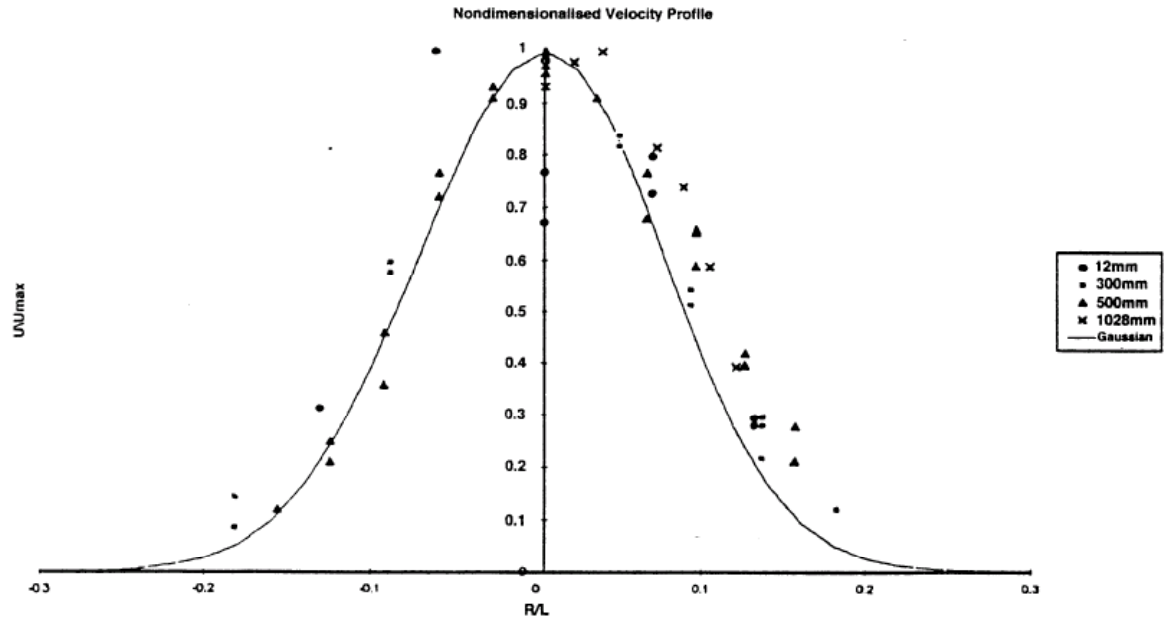


Figure 8. **LDA data of axial droplet velocity for range of downstream distances from release demonstrating self-similar Gaussian profile (Allen)[41]**

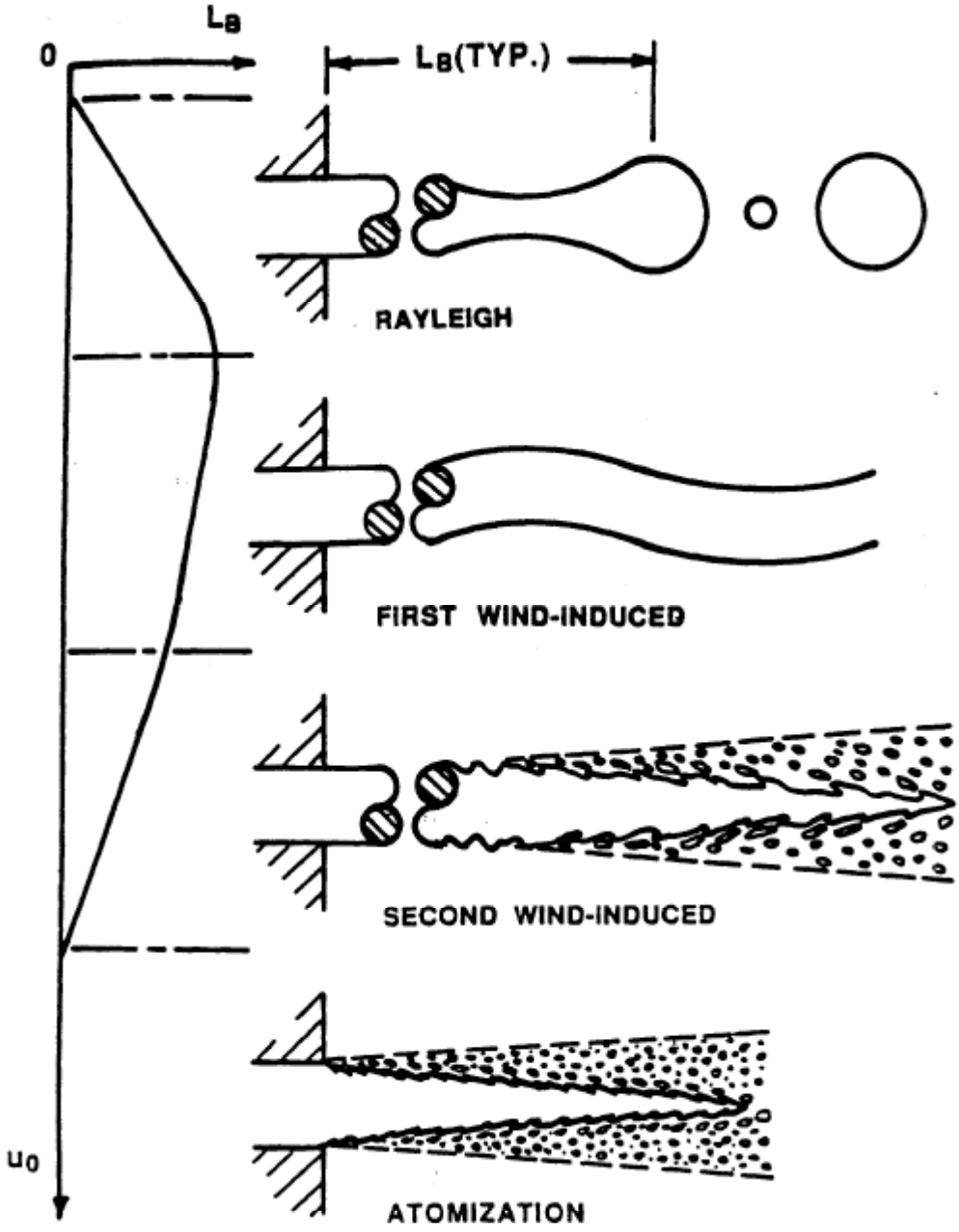


Figure 9. Mechanical jet-break-up regimes (Faeth)[43]

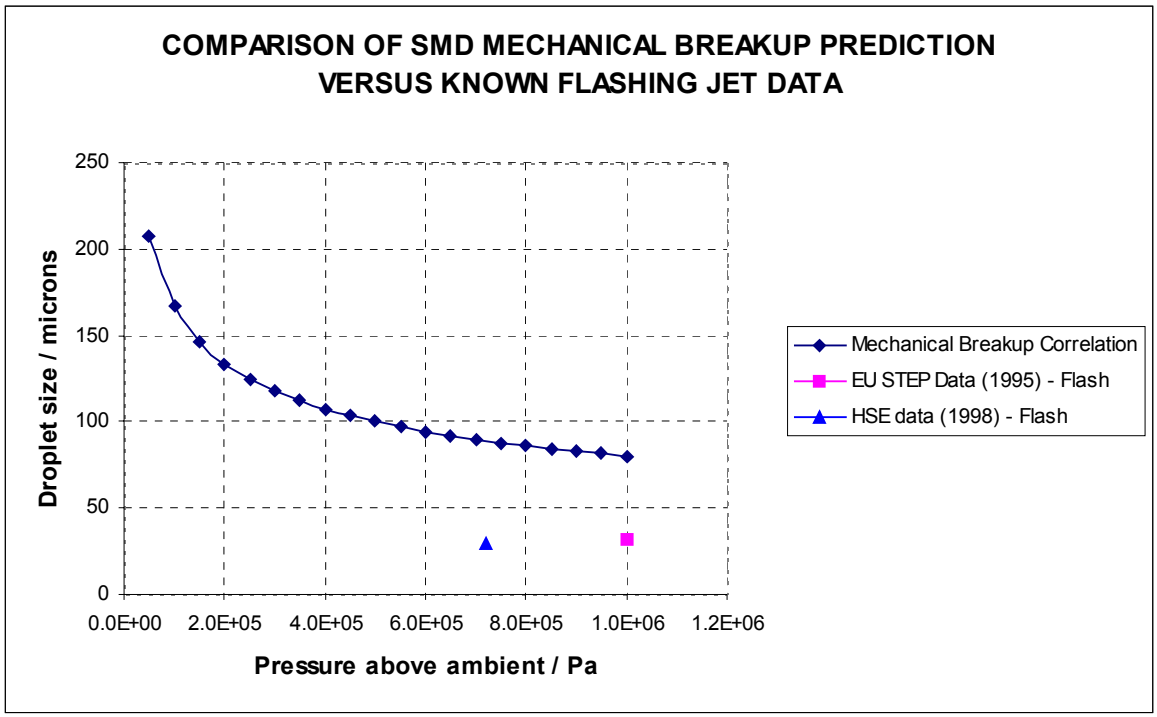


Figure 10. Mechanical break-up mean droplet sizes (Bowen and Maragkos) versus flash break-up

The figure compares the mechanical break-up criterion by Bowen and Maragkos[19] against data points obtained from the EU STEP experiments[14] and HSL experiments by Allen[40].

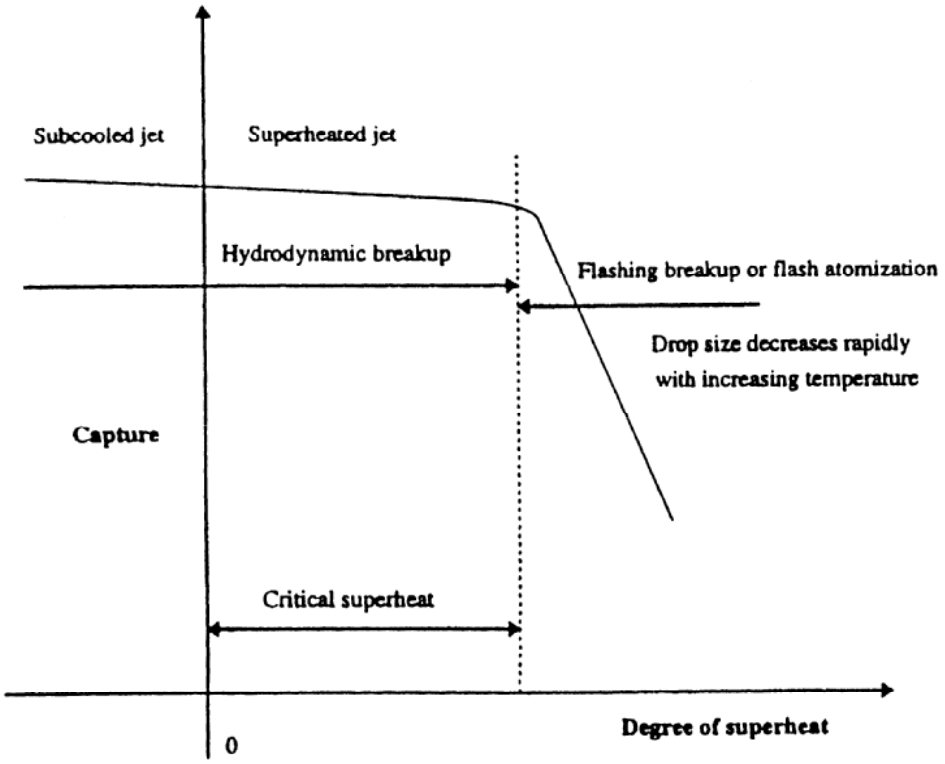


Figure 11. Schematic of flashing and non-flashing regions in relation to rainout (Muralidhar et al.[18])

It is postulated that the droplet size decreases with capture, and therefore the relationship between droplet size and degree of superheat is expected to show a similar trend.

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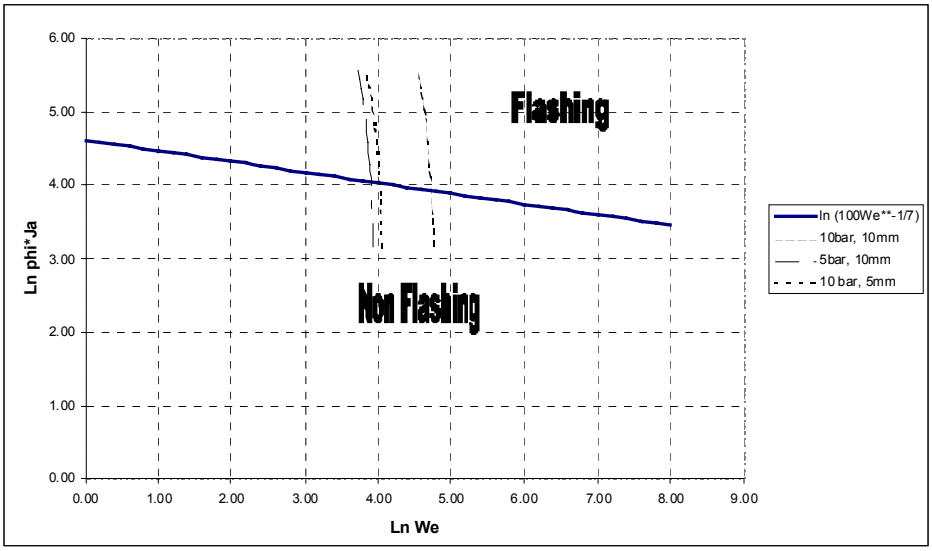

Figure 12. Kitamura[49] transition Criterion

This criterion [Equation (4): phi*Ja = 100 $We^{-1.7}$] governs transition between flashing and non-flashing superheated jets as a function of the Weber number – characterising the fluid dynamics of the jet – and the modified Jakob number phi*Ja = [1- exp(-2300 ρ_v/ρ_L)]Ja – characterising the thermo-dynamic state of the jet. Relevant examples show values required for transition between mechanical and flashing jet break-up.

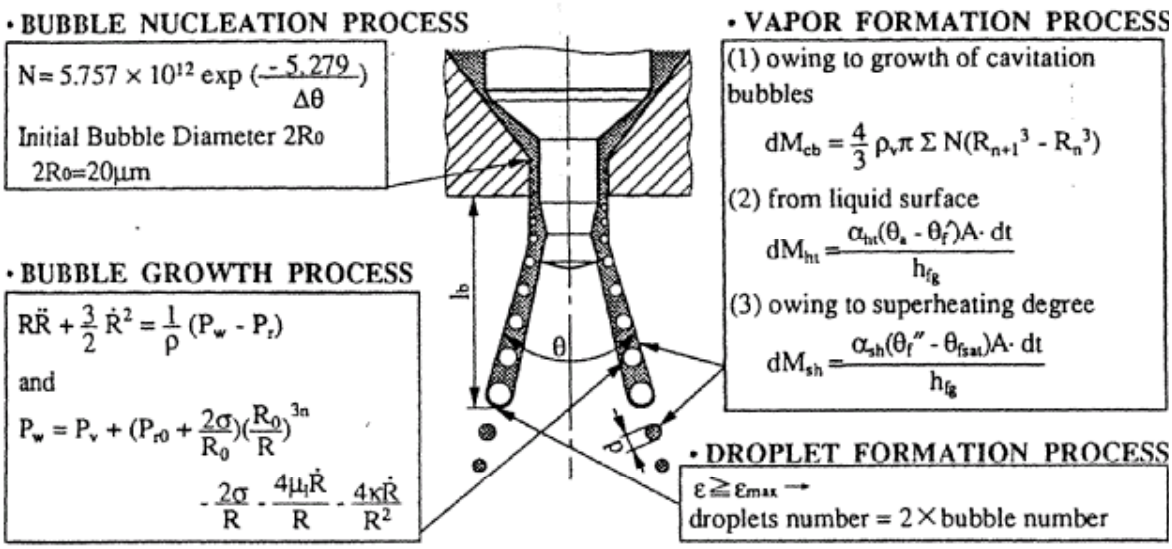

Figure 13. Phenomenological model of flash boiling spray (Fujimoto et al).[61]

Upon release of liquid from nozzle, this figure shows the various phenomenological stages which contribute to the overall atomisation model proposed by these authors. Stages included comprise bubble nucleation, bubble growth, droplet formation and vapour formation, with indication of associated equations and assumptions included within global model.

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