Two-phase jet releases and droplet dispersion: rainout experiments and model validation

Henk W.M. Witlox
DNV Software, 3 Cathedral Street, London SE1 9DE, UK
henk.witlox@dnv.com

Mike Harper
DNV Software, 3 Cathedral Street, London SE1 9DE, UK
michael.harper@dnv.com

Richard Bettis
Health and Safety Laboratory, Harpur Hill, Buxton SK17 9JN, UK
richard.bettis@hsl.gov.uk

Stuart Jagger
Health and Safety Laboratory, Harpur Hill, Buxton SK17 9JN, UK
stuart.jagger@hsl.gov.uk

Phil J. Bowen
Cardiff University
Cardiff University, The Parade, Cardiff, CF24 3TA,Wales, UK
bowenpj@cardiff.ac.uk

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Henk W.M. Witlox
DNV Software
3 Cathedral Street, London SE1 9DE, UK
henk.witlox@dnv.com

Mike Harper
DNV Software

Richard Bettis and Stuart Jagger
Health and Safety Laboratory

Phil Bowen
Cardiff University

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Abstract

Many accidents involve two-phase releases of hazardous chemicals into the atmosphere. This paper describes the results of the fourth phase of a Joint Industry Project (JIP) on liquid jets and two-phase droplet dispersion. The objective of Phase IV of the JIP was to generate experimental rainout data for non-flashing experiments (water and xylene), and to develop recommendations for the best methodology to predict rainout [total rainout mass and its spatial distribution ('distributed' rainout)].

A range of orifice sizes and stagnation pressures were applied. Measurements included flow rate, initial droplet size, plume concentrations/temperatures at a range of downstream locations, and distributed rainout. A photographic technique instead of the PDA method was used which allowed measurement of the larger, non-spherical, droplets. This enabled a more accurate evaluation of the initial droplet size distribution and the initial averaged droplet size (Sauter Mean Diameter, SMD). In addition, still photographs and video records were made of the jets.

Model validation was carried out for the above experiments using two different correlations for the initial droplet size, i.e. the CCPS SMD correlation and the Phase III JIP SMD correlation. The validation includes flow rates, droplet size, distributed rainout, cloud temperature drop and cloud concentrations. Subsequently validation was considered for a wider range of experiments from the literature (sub-cooled and superheated releases) for both SMD and total rainout. Adopted rainout methods comprised both methods including explicit modeling of the droplets (using an extended version of Phast dispersion model UDM), as well as more simple methods based on rainout correlations without droplet modeling. Recommendations are made for most accurate droplet size and rainout modeling.

1. Introduction

Many accidents involve two-phase releases of hazardous chemicals into the atmosphere. Rainout results in reduced concentrations in the remaining cloud, but can also lead to extended cloud duration because of re-evaporation of the rained-out liquid. For accurate hazard assessment one must accurately predict both the amount of rainout and re-evaporation of the pool.

This paper is a summary paper describing the results of a fourth phase of a Joint Industry Project (JIP) on liquid jets and two-phase droplet dispersion. The aim of the project is to increase the understanding of the behavior of sub-cooled (non-flashing) and superheated (flashing) liquid jets, and to improve the prediction of release rate, atomization (initial droplet size after expansion to ambient pressure and before air entrainment), droplet dispersion and rainout. Figure 1 illustrates the consecutive phases in discharge and dispersion. It also shows that droplets of different initial size may rainout at different downwind distances resulting in 'distributed' rainout rather than rainout at a single downwind distance.

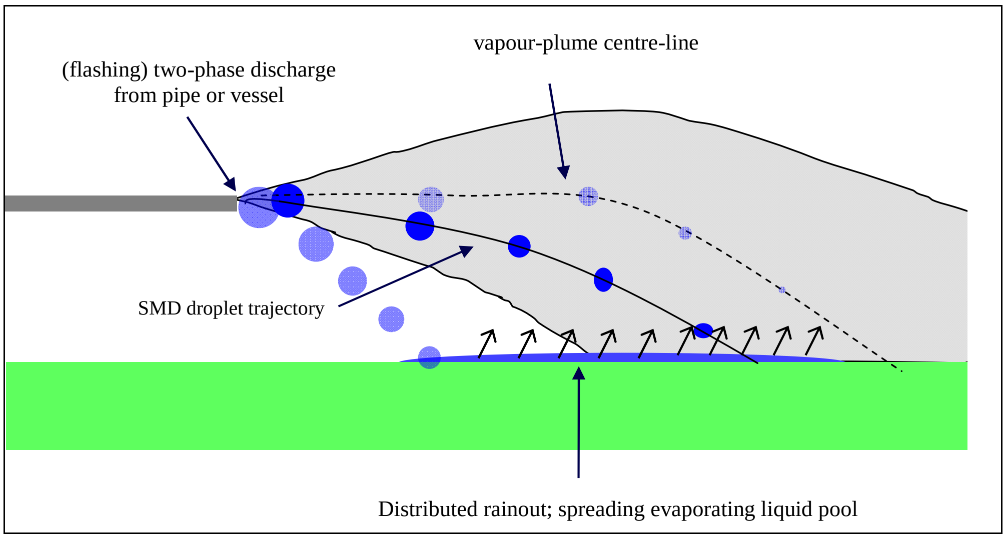


Figure 1. Discharge, droplet dispersion, distributed rainout and re-evaporation

Phase I of the JIP (Witlox and Bowen [1]) governed a literature review on flashing liquid jets and two-phase dispersion. Phase II (Cleary et.. al [2], Witlox et al. [3]) and Phase III (Kay et. al. [4], Witlox et al. [5]) included experimental work limited to measurements of the flow rate and the initial droplet size distribution. The work included:

- Scaled experiments by Cardiff University for a wide range of volatilities (water, cyclohexane, butane, propane and gasoline) with measurements of flow rate and initial droplet size across the full relevant range of superheats. This also included derivation of refined correlations for initial droplet size distribution and Sauter Mean Diameter (SMD).
- Large-scale butane experiments by INERIS (France) to ensure that for more realistic scenarios the derived droplet size correlations are accurate.
- Validation of droplet correlations. New correlations for droplet size distribution and Sauter Mean Diameter (SMD) were implemented into the Phast discharge model. Along with a range of other correlations from the literature, this was validated against JIP experiments and other published datasets. It was shown that the new Phase III JIP droplet size correlation agrees better against experimental data than the existing Phast 6.54 correlation.

- Distributed rainout modeling. The Phast dispersion model (UDM) was also extended to allow simultaneous modeling of a range of droplet sizes. These droplets of different sizes travel along different trajectories and thus predict longitudinal distribution of rainout (rather than at a single point). The new Phase III JIP SMD correlation (without distributed rainout) has been made available as a non-default option in Phast 6.6.

The current Phase IV of the project is a follow-up of Phase III. Its objective is to generate experimental data for non-flashing rainout experiments to validate the new methodology for distributed rainout, and to make refinements where deemed to be necessary:

- Section 2 summarizes the results of the water and xylene rainout experiments carried out by the Health and Safety Laboratory (HSL). These experiments involved indoor sub-cooled water and xylene jets with a range of nozzle diameters and source pressures. Measurements were carried out of release rate, initial droplet size distribution, distributed rainout, concentrations and temperatures.
- Section 3 summarizes the results of model validation and model improvements by DNV Software. This validation was carried out using extended versions of the discharge and dispersion models in the Phast hazard assessment package. This validation included validation against the HSL experiments. It also includes validation for a wider range of experiments for both SMD and total rainout. A range of initial droplet size correlations and rainout methods was applied, and recommendations for the best method of modeling are formulated.
- Section 4 summarizes the main conclusions and recommendations for further work.

2. Water and xylene rainout experiments

The first part of the Phase IV work included water and xylene rainout experiments by HSL. The work was carried out indoors to avoid added complications associated with weather fluctuations. Experiments were carried out using sprays of water and xylene from nozzles of 2.5 mm and 5.0 mm diameter and at source pressures from 4 barg to 16 barg; see Figure 2.

Alongside measurements of the release conditions and flow rates, measurements were made of the amount and downstream position of rainout from the jets (distributed rainout), droplet size within the jet using direct visualization and, for xylene, the temperature of the jet and the concentration of xylene within it. In addition, visual records were made of the jets. These included still photographs of the early part of the jet, and a video record of the xylene jet under each set of release conditions. For a selected number of experiments, an estimate of the jet break-up length was obtained from the photographs.

In the preceding phases II and III of the JIP a PDA (Phase Doppler Anemometry) technique was applied. However this method ignores non-spherical droplets and cannot measure larger droplet sizes. Therefore for the current phase IV a photographic technique instead of the PDA method was applied to include measurement of the larger (non-spherical) droplets. This enabled a more accurate evaluation of the initial droplet size distribution and the initial averaged droplet size (Sauter Mean Diameter, SMD). The results showed that that the droplet behavior in the jet is more complex than had been anticipated with a few large non-spherical droplets accounting for a large proportion of the mass; see Figure 3 for a selected water experiment. Consequently a large number of spray images was required to evaluate an accurate droplet mass size distribution.

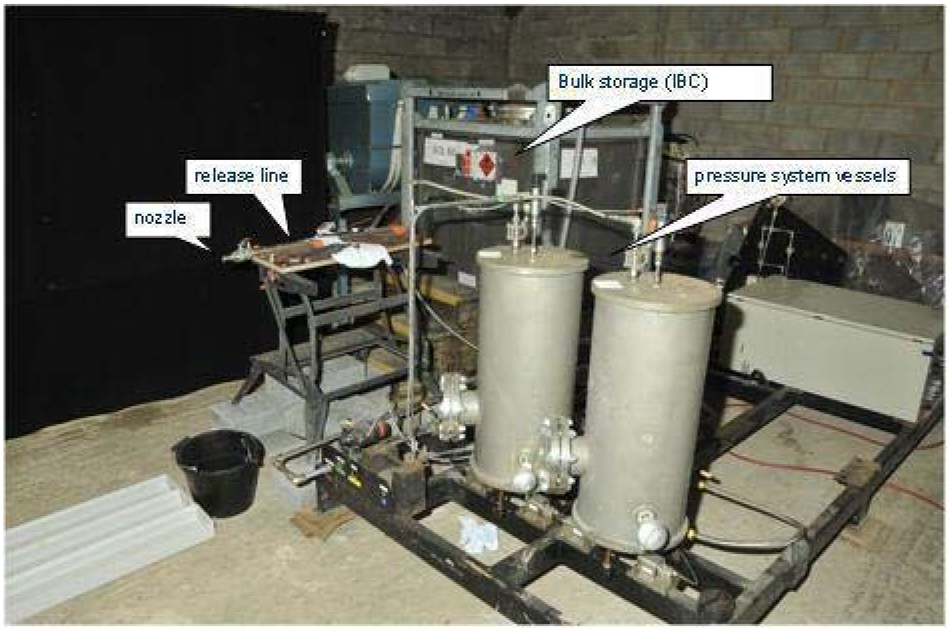
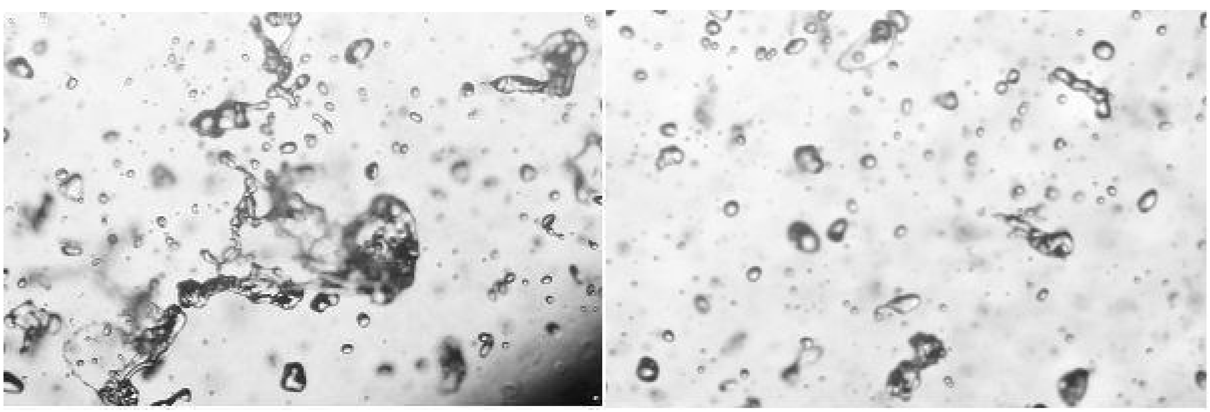


Figure 2. Experimental rig



(a) 1.25m downstream (500 diameters) (b) 2.5m downstream (1000 diameters)

Figure 3. Droplet size images (water experiment, 2.5 mm nozzle, 10barg)

Distributed rainout was measured by weighing the amount of rainout in trays positioned along the jet direction as shown in Figure 4. The rainout results showed a good degree of repeatability and internal consistency. They indicated that an increasing proportion of the released material did not rain out for increasing pressure (over 10% for the larger pressures for the xylene experiments). Rainout distance also increased with increasing pressure. The cooling effect of the evaporation of the liquid was confirmed by the xylene temperature results.

Figure 4. Distributed rainout measurements

3. Model validation

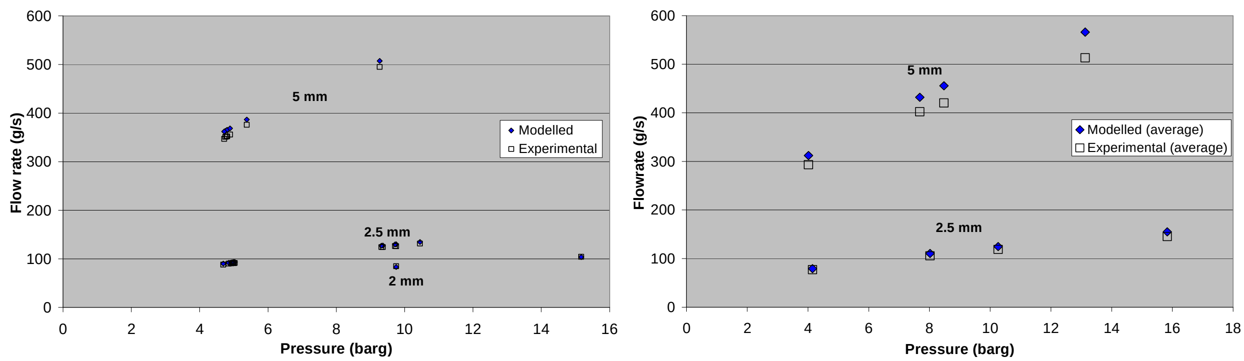
2.1 Introduction

The second part of the Phase IV work included model validation and model refinements by DNV Software. This included validation of the Phast discharge model DISC [flow rate; post-expansion droplet size (Sauter Mean Diameter, SMD)] and the Phast dispersion model UDM [distributed rainout, temperatures and concentrations].

Secondly validation against the above HSL water and xylene experiments was carried out. In this paper we will report validation against HSL measurements for flow rate, initial droplet size and rainout. The validation for droplet size and rainout will also be summarized for a wider comprehensive set of experiments available in the literature. Details of the validation against the HSL concentrations and temperatures will be reported in a future paper.

2.2 Flow rate

In the discharge calculations the liquid was modeled as an incompressible liquid for both the water and xylene experiments. Figure 5 shows that very close agreement of the flow rate observed in the HSL experiments was obtained. It also demonstrates the increase of flow rate with increasing pressure and increasing nozzle diameter.



(a) water (b) xylene

Figure 5. Validation of flow rate for HSL water and xylene experiments

2.3 Droplet size

The validation was carried out using four different correlations for the initial droplet size (SMD).

- the *original CCPS* correlation, where the SMD (m) is taken as the minimum of the value d_{da} derived from a mechanical break-up criterion (based on critical Weber number) and the value d_{df} derived from a flashing break-up criterion.
- a *modified CCPS* correlation is applied with the mechanical break-up value d_{da} applied for sub-cooled jets and the flashing break-up value d_{df} for superheated releases.
- the *Melhem* correlation based on a Weber number criterion generalized for superheated liquids
- the *Phase III JIP* correlation defined the SMD as a reducing tri-linear function of superheat with the initial regime governed by mechanical breakup, an intermediate transition regime, and a final regime governed by fully flashing break-up. This correlation also includes a correlation for the droplet size distribution based on the Rosin-Rammler droplet size distribution.

See Witlox et al. [5] for full details of the above correlations. Figure 6 includes validation against the water experiment for which images were shown in Figure 3. It is seen that the Phase III JIP initial droplet size distribution correlation closely matches the droplet size distribution observed at 500 diameters distance. It is also apparent that further downstream (at 1000 diameters) droplets are smaller because of secondary break-up of non-spherical droplets. The same qualitative behavior can be seen in Figure 3.

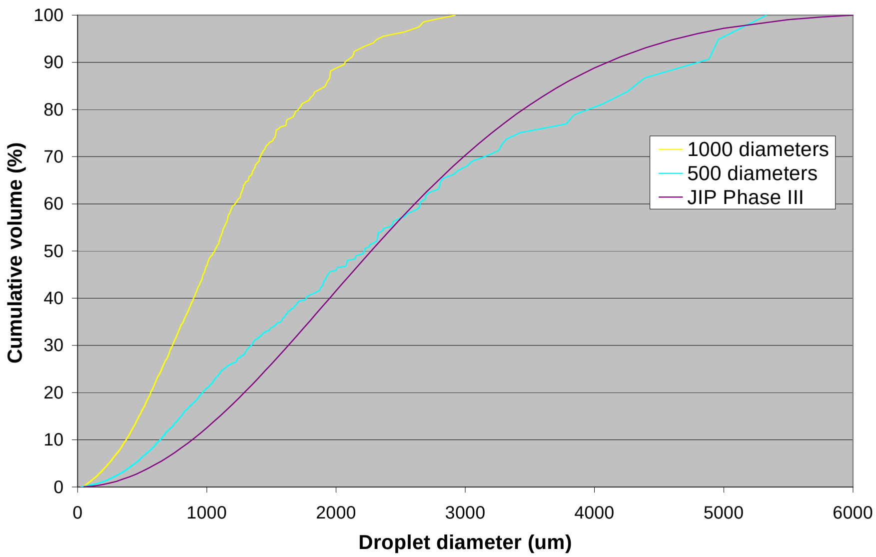
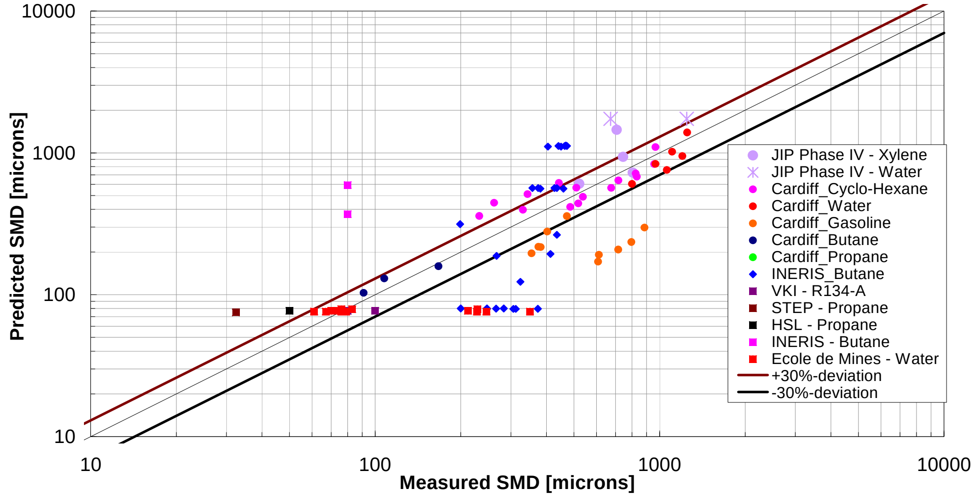
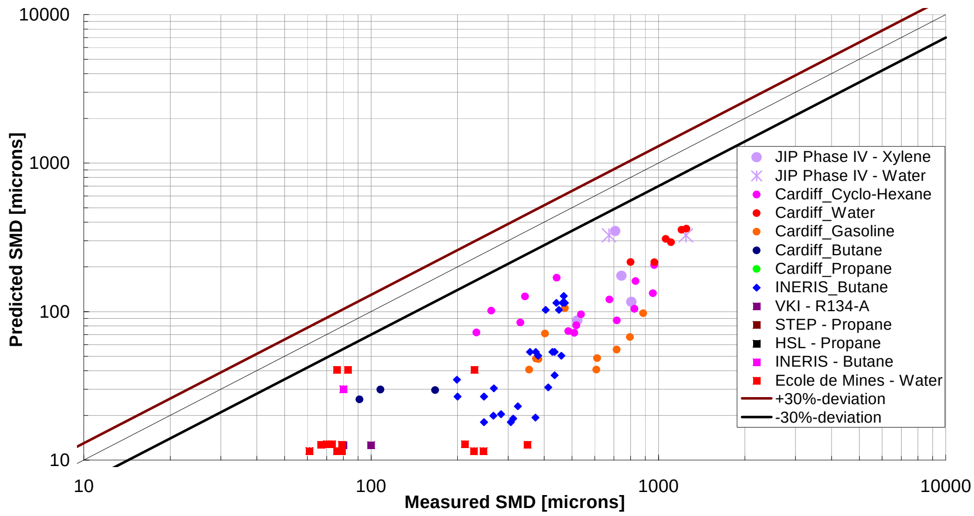


Figure 6. Validation of droplet size distribution (water experiment, 2.5mm nozzle, 10barg)

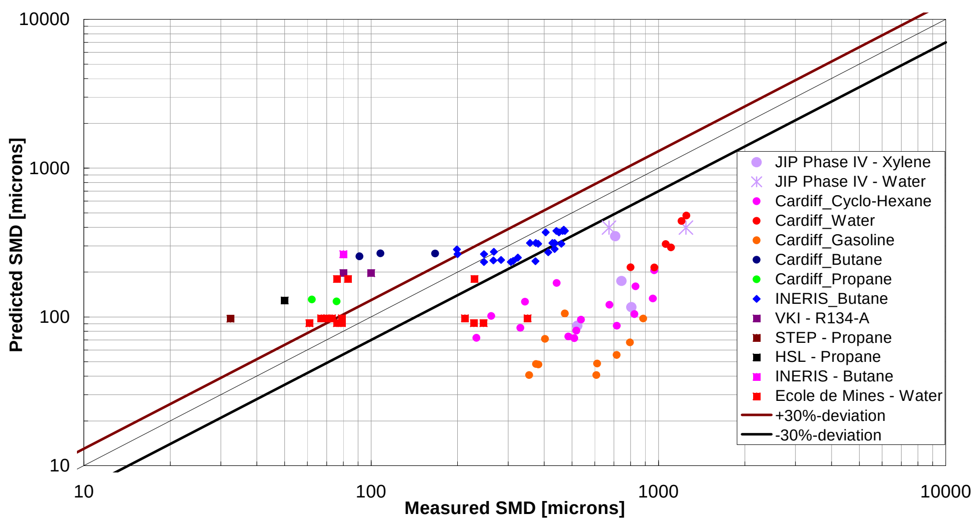
Figure 7 includes validation results for initial droplet size (SMD) for a comprehensive set of experiments, i.e. the Phase IV JIP experiments (water and xylene), Phase III JIP experiments (Cardiff and INERIS experiments) as well as other experiments available from the literature: the STEP propane (Hervieu and Veneau, [7]), the VKI R134-A (Yildiz et al., [8]), the HSL propane (Allen, [9]), Ecole de Mines water and INERIS butane (Touil et al, [10]) experiments. The Phase III JIP correlation is seen to perform best against the set of experimental data studied. The original CCPS correlation generally under-predicts since it takes the minimum of the mechanical and flashing droplet size correlation regardless of the degree of superheat, while the modified CCPS correlation shows improved results.



(a) Phase III JIP SMD correlation



(b) Original CCPS correlation (Phast 6.6 default)



(b) Modified CCPS correlation (Phast 6.7 default)

Figure 7. Validation of SMD droplet size correlation against sub-cooled experiments

2.3 Rainout

The UDM outdoor dispersion model in Phast allows for two-phase dispersion including droplet modeling, rainout of the droplets to form a pool, pool evaporation and subsequent addition of vapor back to the cloud; see Figure 1. The JIP III correlation predicts a distribution of droplet sizes (see Figure 6) and the UDM model was extended to use this distribution by modeling a discrete set of droplet sizes (or droplet parcels). Each parcel therefore follows its own trajectory in the cloud and rainout is distributed in the downwind direction; see Witlox et al. [5] for full details of the model.

Figure 8 depicts the validation of the UDM results against a selected xylene experiment for a range of droplet size correlations. A single droplet size (SMD) with rainout at a single point was modeled for the CCPS (there was no difference in this case between modified and original CCPS) and Melhem correlations. For the Phase III JIP droplet size correlation the initial droplet size distribution was modeled by twenty droplets (based on equal-mass parcels) with increasing droplet size. It is seen that the Phase III JIP correlation predicts too much rainout over too narrow a rainout zone. The other two correlations predict all rainout at a single point, and is seen that the CCPS correlation most accurately predicts the total amount of rainout. The above conclusions were found to be valid for the overall set of HSL experiments.

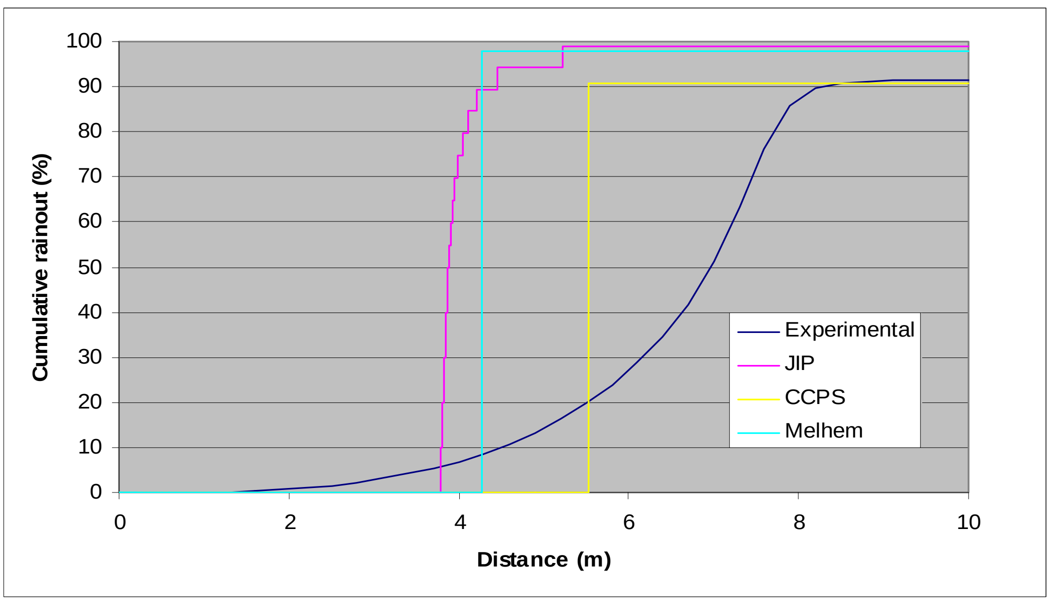


Figure 8. Validation of rainout model against HSL xylene experiment (2.5 mm nozzle, 8barg)

The extended Phast discharge and dispersion models (DISC, UDM) have been validated against a subset of the CCPS experiments (two tests randomly chosen for each of the five chemicals (water, CFC-11, chlorine, cyclohexane and monomethylamine). See Johnson and Woodward [6] for full details on the CCPS and MMA Rohm and Haas rainout experiments. Figure 9 includes the measured (uncorrected) rainout results as well as measured rainout 'corrected' to account for evaporation. UDM results are provided for the JIP III correlation both without parcels (model SMD droplet only) and with droplet parcels, as well as for the CCPS correlation (original and modified).

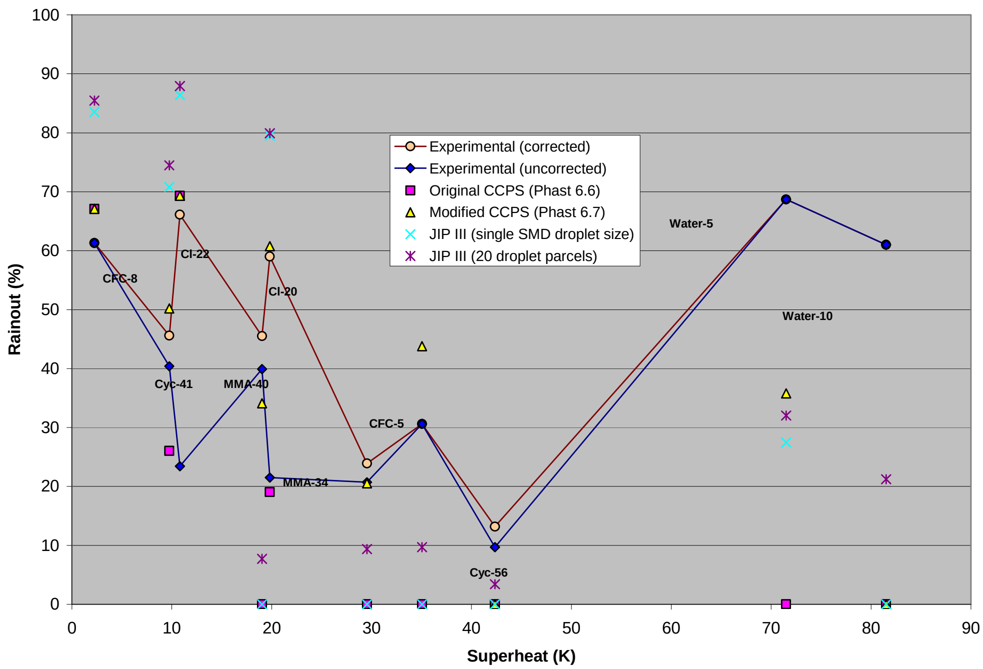


Figure 9. Validation of rainout model against CCPS experiments

Figure 9 demonstrates the over-prediction of the rainout at low superheats by the Phase III JIP correlation (because of too large initial droplet size), the under-prediction of rainout by the original CCPS correlation (because it erroneously picks up the initial mechanical breakup droplet size instead of the flashing break-up size). The best predictions are provided by the modified CCPS correlation, but it must be noted that it is based on the flashing CCPS droplet-size criterion derived from a best fit against the corrected rainout for the CCPS experiments.

Validation was also carried out for other two-phase elevated releases for which little or no rainout was measured, i.e. 2-phase elevated releases from the existing UDM validation dataset (EEC propane, Desert Tortoise and FLADIS ammonia, Goldfish HF).

In addition to the above UDM rainout methods (including explicit modeling of the droplets), also more simple rainout methods were applied based on rainout correlations without droplet modeling. This included rainout correlations by DeVaull and King [11] and Lautkaski [12].

4. Conclusions

A small number of large non-spherical droplets contribute to a large mass fraction of the overall mass for sub-cooled releases. Therefore a large number of images are required to obtain an accurate initial droplet size volume distribution. Secondary droplet breakup is seen to occur.

From the above validation (for all methods and all experiments), it is concluded that the modified CCPS droplet size correlation provides the overall best prediction of rainout, while the Phase III JIP droplet size correlation provides the best overall prediction of initial droplet size. The UDM rainout methods were overall shown to be superior to the simpler rainout methods. More details of this are planned to be published in a separate paper.

5. Future work

A literature survey, validation and possibly improved modeling is recommended for post-expansion modeling (velocity and liquid mass fraction) and near-field jet dispersion modeling, possibly together with some limited experimental work as necessary. This would complement previous JIP validation work associated with flow rate, and post-expansion droplet size modeling. Also additional rainout experiments are recommended for both sub-cooled releases (at larger scale) and flashing releases (including pool re-evaporation). At a later stage, additional work could be related to multi-component releases to study the effect of release of mixtures. This could include further improvement of multi-component modeling (droplet modeling and pool evaporation).

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