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Sub-cooled and flashing liquid jets and droplet dispersion I. Overview and model implementation/validation

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ABSTRACT

Many accidents involve two-phase releases of hazardous chemicals into the atmosphere. This paper describes the results of a third 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 behaviour of sub-cooled non-flashing and superheated flashing liquid jets, and to improve the prediction of initial droplet size, droplet dispersion and rainout.

Phase III of the JIP first included scaled experiments for materials with a range of volatilities (water, cyclohexane, butane, propane and gasoline). These experiments were carried out by Cardiff University including measurements of flow rate and initial droplet size across the full relevant range of superheats. See the companion paper II for further details of these experiments and the derivation of new refined correlations for droplet size distribution and Sauter Mean Diameter. Furthermore large-scale butane experiments were carried out by INERIS (France) to ensure that for more realistic scenarios the derived droplet size correlations are accurate.

Model validation and model improvements were carried out by DNV Software, including validation of release rate and initial droplet size against the above scaled and large-scale experiments. New correlations for droplet size distribution and Sauter Mean Diameter (SMD) were implemented into the Phast discharge model. These were compared against a range of other droplet size and rainout correlations published in the literature, in conjunction with validation against an extensive set of experiments. It was shown that the new droplet size correlation agrees better against experimental data than the existing Phast correlation. To further improve the rainout prediction, the Phast dispersion model (UDM) was also extended to allow simultaneous modelling of a range of droplet sizes and distributed rainout (rather than rainout at one point).

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 describes the results of a third 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 behaviour of sub-cooled (non-flashing) and superheated (flashing) liquid jets, and to improve the prediction of release rate, atomisation (initial droplet size), droplet dispersion and rainout.

Phase I of the JIP was carried out by Witlox and Bowen (2002) and involved a detailed literature review on flashing liquid jets and two-phase droplet dispersion. The review considered models and validation data for the sub-processes of droplet atomisation, atmospheric expansion to ambient pressure, two-phase droplet dispersion, rainout, pool formation and re-evaporation; see Fig. 1. Phase II of the JIP included water experiments from low-superheat non-flashing jets to high-superheat fully flashing jets (Cleary, Bowen, & Witlox, 2007). The experiments measured velocity and droplet size distribution close to the orifice (post-expansion data) in order to derive an improved droplet size correlation valid for release conditions. A criterion was derived for the transition between 'low' and 'high' superheat (non-flashing jets and fully flashing jets), and initial droplet size correlations were proposed in the regimes for non-flashing (mechanical break-up), transition to

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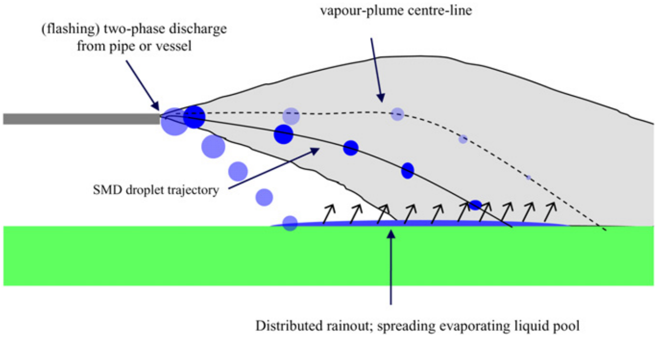

Fig. 1. Modelling of droplet dispersion, distributed rainout and re-evaporation.

flashing and fully flashing. The Phase II JIP droplet size correlation was compared with previous correlations from the literature (Witlox, Harper, Bowen, & Cleary, 2007). This also included detailed validation for both initial droplet size and rainout.

Phase II was limited to scaled experiments for water with initial droplet-size data measured at a single value of the superheat only. Furthermore the modelling simplistically assumed one single averaged droplet size (Sauter Mean Diameter, SMD) with rainout at a single point only. As a result, Phase III was initiated to account for these issues. The current paper provides an overview of the Phase III results.

Phase III of the JIP first included scaled experiments for materials with a range of volatilities (water, cyclohexane, butane, propane and gasoline). These experiments were carried out by Cardiff University including measurements of flow rate and initial droplet size across the full relevant range of superheats. It provided recommendations for initial droplet size correlations in the regimes of mechanical break-up, transition to flashing, and fully flashing, and the tri-functional modelling approach previously proposed in Phase II of the JIP was endorsed. The reader is referred to the companion paper (Kay, Bowen, & Witlox, 2010) for further details.

Section 2 includes Phase III results of large-scale butane experiments, which were carried out by INERIS (France) to ensure that for more realistic scenarios the derived droplet size correlations are accurate. Section 3 describes in detail the newly derived Phase III SMD correlation as well as previous correlations from the literature. Section 4 includes Phase III results of discharge model improvements and validation carried out by DNV Software, including validation of release rate and initial droplet size against the above scaled and large-scale experiments. Section 5 describes dispersion model improvements and validation. This includes simultaneous modelling of a range of droplet sizes and distributed rainout (Fig. 1) rather than rainout at one point. This approach is validated against CCPS rainout experiments (Johnson & Woodward, 1999).

2. Large-scale butane experiments

In addition to the small-scale experiments by Cardiff University, Phase III also included large-scale butane experiments by INERIS. These were carried out to ensure that for more realistic scenarios the derived droplet size correlations are accurate.

Fig. 2 illustrates the experimental rig for one of the large-scale butane experiments. Both flow rate and PDA droplet-size measurements were carried out.

Six experiments were carried out using butane of purity 99.5%. Table 1 includes the corresponding test matrix. It is seen that the experiments include a range of orifice sizes (5, 10 and 15 mm; negligible L/d ratios), release pressures (2, 6 and 10 barg), and superheats (7–27 °C). Measurements taken include ambient data

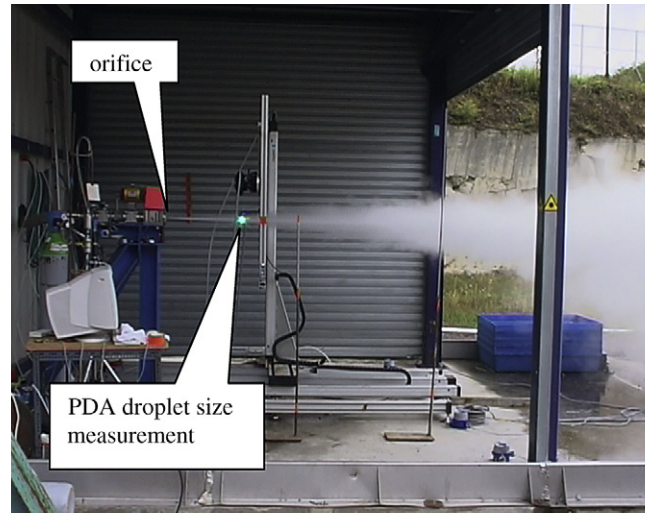

Fig. 2. PDA droplet size measurement for large-scale butane experiment (INERIS).

(temperature, pressure), tank data (weight, pressure and temperature as function of time), data immediately upstream of the orifice (pressure and temperature as function of time) and PDA droplet size measurements. Table 1 includes the axial distances at which data were taken at a range of ‘crosswind’ distances (0, ±3, ±6 cm; distances on a horizontal line perpendicular to the axial direction). It also includes the maximum droplet size d_{max} that could be measured (700–800 μm). This was considered to be a sufficient range for the distribution of number of droplets, but larger droplets may be missed resulting in a possibly inaccurate droplet volume distribution. The number of droplets at each PDA measurement location was typically in the range between 2000 and 20,000 droplets.

Fig. 3 includes the droplet size distribution data for one of the INERIS experiments. Like for the Cardiff experiments (see companion paper II), it is observed that some data may be ‘clipped’, i.e. for some cases there are possibly droplets larger than those actually measured.

See Section 4 for details of the model validation of the flow rate and the droplet size (SMD) against the above INERIS experiments.

3. Overview of droplet-size correlations

Witlox et al. (2007) previously provided an overview of correlations for the Sauter Mean Diameter (SMD) of the droplet size.

The original SMD correlation in Phast is the Weber/CCPS correlation proposed by Johnson and Woodward (1999), where SMD (m) is taken as the minimum of the value d_{da} derived from a mechanical break-up criterion (based on critical Weber number We_{crit}) and the value d_{df} derived from a flashing break-up criterion (reducing with partial expansion energy E_p, J/kg).

Table 1
Test matrix for large-scale butane experiments (INERIS).

Number of experiment	Orifice diameter (mm)	Release pressure (barg)	Release temperature (C)	PDA axial distances (cm)	PDA resolution d_{max} (μm)
1	5	6	15–26	60	700
2	10	6	26–27	60,85	800
3	10	10	19–22	60,85	800
4	15	6	17–21	60,85	750
5	10	6	9–10	40,60,85	750
6	10	2	7–9	40,60,85	750