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Modelling Small-scale Flashing Propane Jets

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Accidental releases of pressure liquefied materials may result in instantaneously vaporising, or flashing, jets which mix with ambient air and disperse. In consequence modelling, it is important to correctly describe the initial jet behaviour as this can influence the subsequent vapour dispersion. Numerous techniques are available for modelling flashing jets and their dispersion and Computational Fluid Dynamics (CFD) is a tool that is becoming more widely used. Confidence in model predictions can be gained by comparing them with experimental data as well as with other models. This paper describes the CFD modelling of a small-scale flashing propane jet and comparison with both experimental data and integral model predictions.

1. Introduction

In assessing the consequences of a release of a pressure liquefied gas, flashing jet models are often used to provide the input, or source term, for vapour dispersion calculations. That is, the flashing jet model encompasses the initial discharge, rapid expansion, mixing and vaporisation. The output from these calculations forms the source term which can be used as the input to an atmospheric dispersion model which then determines the subsequent dispersion of the gas cloud. The function of the flashing jet model is to estimate a source term typically comprising the temperature, velocity, concentration and the liquid fraction using the initial storage conditions, leak dimensions and material properties.

Flashing jet modelling is usually generalised into several stages. Firstly, an estimate of the discharge conditions at the exit from the pipe or vessel; secondly, a description of the initial liquid expansion to atmospheric pressure; and finally, the dispersion of the two-phase mixture into air, where the droplets evaporate into vapour. While these stages aim to capture observed behaviour, they are chosen as much for modelling convenience as for physical reasons. A number of flashing jet models have been developed and these range from simple expressions, through integral (whole jet) models to Computational Fluid Dynamics (CFD) simulations. Each approach has its strengths and weaknesses, and the robustness of each model needs to be carefully checked (validated) by comparison with experimental data.

2. Small scale flashing experiments

Numerous experimental studies have been undertaken to examine flashing releases and these can be broadly classified into dispersion experiments at both laboratory and field scale and discharge experiments. Bricard and Friedel (1998) provide an overview of dispersion experiments and also of the various modelling approaches in use at the time. Historically, many of the discharge experiments have been undertaken to determine flow rates from pipes, orifices and tubes to provide data for models of pressure relief and venting systems, in addition to determining source terms for dispersion modelling. Examples of discharge experiments are given by Fletcher (1984) and Richardson *et al.* (2006) and a review of experimental data is given by Polanco *et al.* (2010). In many studies available in the public domain, measurements were concerned with either the discharge rate or the far-field dispersion and relatively few attempted to measure the properties of the jet near the exit. This is likely to be in part due to the difficulty of making any type of accurate measurements in a flashing two phase flow.

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An exception is the small scale measurements in flashing jets by Allen (1995) who conducted experiments on releases of propane at saturation conditions through 4 mm diameter, 40 mm length pipes. Initially, measurements of temperature were made using thermocouples, but the measurement programme was later extended to include velocities. The details of the experiments are given in Table 1 and were obtained from the data report of Allen (1995) and a report on one-dimensional modelling by Tickle *et al.* (1997).

Table 1: Test parameters

Parameter	Value
Material	Propane
Hole diameter (mm)	4
Pipe length (mm)	40
Ambient temperature (K)	288.8
Storage temperature (K)	288.8
Pressure (barg)	6.47
Measured release rate (g/s) (average over all tests)	84.3

3. Flashing jet models

Many models are available for estimating hazard ranges from flashing releases, though for a given orifice size, calculation methods which provide conservative predictions (i.e. underestimation) of the flow rate through relief valves will tend to be non-conservative when applied to leak and dispersion scenarios. Wheatley (1987) describes a model for determining the jet properties from flashing releases of ammonia including the thermodynamics of mixing ammonia with atmospheric moisture. The EJECT model of Tickle (1997) is also an integral model for flashing jets which was subsequently incorporated into the DRIFT 3 (Tickle and Carlisle, 2008) gas dispersion model. Computational Fluid Dynamics (CFD) has successfully been used to simulate the dispersal stage of flashing jets (Kelsey, 2001, Dixon *et al*., 2012) however, in both cases, the simulations were started after the flashing depressurisation region and an additional model was used to carry out the initial flashing calculations. A review of techniques that have been applied to modelling flashing releases is given by Britter *et al*. (2011), covering both pure liquid and two-phase discharge from various sources such as pipes, tubes and cracks. One of the main difficulties in modelling orifice type flashing flows is the uncertainty surrounding the conditions at the exit and many of the experimental studies did not capture the flow detail in this region.

In the present work, three different integral models have been tested: DRIFT 3.7.2, Phast 6.7 and QUADVENT 1.9.9.17. ESR Technology's DRIFT (Dispersion of Releases Involving Flammables or Toxics) model was developed for the UK Health and Safety Executive (HSE) in the 1990s and more recently updated to DRIFT 3. DRIFT 3 can model ground-based or elevated clouds, released either instantaneously or as a steady continuous source, and it incorporates a jet model to predict dispersion from pressurised releases. DNV Phast (DNV, 2011) is a general purpose consequence modelling tool that incorporates models to describe the depressurisation, flashing and dispersion process. QUADVENT (Webber *et al.,* 2011) is a tool for carrying out area classification studies, developed by the Health and Safety Laboratory (HSL). It was originally developed for modelling gas jets but has recently been updated to model flashing liquid releases. The main difference between QUADVENT and other dispersion models is its capability to model indoor releases in nil wind and to account for the accumulation of gas in an enclosed space. Simulations have been performed using DRIFT 3 and Phast both with and without humidity effects.

4. CFD modelling

The general purpose CFD code, ANSYS CFX 15 (ANSYS, 2013) has also been used to model the jet from the point at which it has expanded to atmospheric pressure. Detailed modelling of the initial discharge and flashing process was not attempted, as this is not routinely carried out with CFD in consequence modelling applications. Determining the break-up of a liquid stream into droplets is extremely challenging for non-flashing jets and the models developed for this tend to be aimed toward the type of flow found in automotive fuel injection systems. DNV Phast was therefore used to model the initial expansion process and the post-expansion conditions were applied as input to the CFD model as given in Table 2. CFD was used to model the spray of liquid droplets, their subsequent evaporation and the dispersal of vapour in the jet. To do this, the CFD model used an Eulerian-Lagrangian approach, in which there is a computational mesh fixed in space through which the vapour flows. Momentum, mass and energy conservation equations are solved in each mesh cell to find the velocity, temperature, pressure and concentration distributions. The spray of droplets was modelled using Lagrangian particle tracking. The paths of discrete computational particles are tracked through the flow domain from their injection point until they hit a solid surface, escape the domain or evaporate completely.

Table 2: Post-expansion values from DNV Phast

Post-expansion condition	Value
Predicted mass flow rate (g/s)	69.2
Velocity (m/s)	124.56
Temperature (°C)	-42.07
Liquid fraction (-)	0.69
Mass flow of droplets (g/s)	47.8
Expanded diameter (mm)	9.6
Droplet diameter (μm)	193 (modified CCPS correlation)

4.1 Geometry and meshing

The domain consisted of a cylinder 2 m in diameter by 4 m long with a cylindrical pipe section equal to the expanded diameter protruding 40 mm from one of the circular end faces. The domain was meshed using tetrahedral cells, with a near wall inflation layer of prismatic cells applied to the pipe surfaces. Six meshes were created with between 0.1 and 4.2 million nodes, which were each refined in the vicinity of the jet.

4.2 Input parameters

The CFD model was run with the following input parameters:

- Liquid phase Lagrangian particles injected at the end of the pipe with a co-flow of vapour
- Domain ends and sides set as openings with zero gradient turbulence
- Shear Stress Transport (SST) turbulence model (Menter, 1994)
- Reitz and Diwakar particle breakup model (Reitz and Diwakar, 1987)
- Initial conditions of a low but finite turbulence intensity
- Turbulence of the vapour phase set according to the inlet velocity the expanded diameter

A simple one-at-a-time sensitivity analysis was also carried out where a range of values were used for a subset of the input parameters shown in Table 3.

Table 3: Ranges of input parameters varied

Parameter	Value
Number of particles	10000, 5000, 2500
Particle initial diameter (μm)	193, 100, 20
Timestep (s)	0.5
Particle iteration frequency	3
Number of particle integration steps per element	50, 25, 10
RMS residual target	1E-5

4.3 Post processing

Allen (1995) presents the temperature measurements as both a minimum temperature and an average over a steady period. The temperature measurements were made using bare thermocouples and so in a flashing two phase jet may represent the combination of several different physical processes. Liquid droplets may impact on the thermocouple, evaporate and cause it to register a low temperature or water condensed from the atmosphere may form a layer of ice. Furthermore, measurements made by arresting a high speed flow will tend to be slightly higher than those made non-invasively, though this effect is likely to be fairly small (in the order of a few K) for the flows under consideration. The temperature measurements therefore will represent a mass average between the continuous and liquid phases. For the CFX results, two temperatures were extracted: the centreline vapour phase temperature on the Eulerian mesh and a liquid temperature. The latter was computed by mass-averaging the particle temperatures along the centreline of the jet.

4.4 Results

Figure 1 is a comparison of the overall temperature predictions with the measured values from Allen (1995). Temperatures are plotted against the downstream distance, x, normalised by the nozzle diameter, D. In all the models, the initial flashing expansion region is assumed to have negligible distance and the results are shown from the point where atmospheric pressure is reached and the liquid is at its boiling point. The CFD results are taken from the least “expensive” simulation – the coarse 0.1 million node mesh with 2,500 particles and 10 integration steps per element and the smallest particle size of 20 μm. The predicted liquid temperatures are shown in red by the error bars representing the maximum, minimum and average over all the particles at each location. The experimental measurements obtained from Allen (1995) are plotted as a minimum value and an average minimum. In the region where there are droplets present, it is likely that the measurements are biased towards the droplet temperature and it is therefore appropriate to compare with the CFD predicted liquid temperatures. On this basis, the CFD results are in reasonable agreement with the experiments in the region where liquid is present. The temperatures are initially slightly overpredicted and the lowest temperature is slightly underpredicted. The CFD model predicts the persistence of the droplets well, but the difference between the liquid and vapour temperatures shows that equilibrium is not reached, even with the small 20 μm droplets. In the region of the jet after all the liquid has evaporated, all the models slightly underpredict the temperature rise, In this region, QUADVENT, DRIFT 3 and Phast gave similar results but the DRIFT 3 and Phast predictions including the ambient humidity were more accurate, due to the heat released from condensation. Using the larger initial particle diameter in the CFD model moved the liquid temperature further away from equilibrium but this did not influence the far-field temperatures, velocity or concentration significantly.

Figure 2 compares the vapour phase velocities for the four models against the measurements. Good agreement is obtained across the models and the measurements for values of x/D greater than about 100. Up until this point, the measurements suggest a discharge velocity of about one third of that predicted. The reason for this may be due to the uncertainty of the state of the material leaving the orifice. Two phase flows tend to be highly compressible and if flashing occurs in the pipe, the discharge velocity would be limited by choking at the exit. For consequence modelling, it is ultimately the predicted concentrations that are of interest and, as shown in Figure 3, all the models result in very similar predictions by x/D of 500, where the concentration is approximately 0.05 mol/mol. The integral models (which all assume homogeneous equilibrium) produce similar concentrations to the CFD model, over all the ranges of parameters tested in the CFD model.

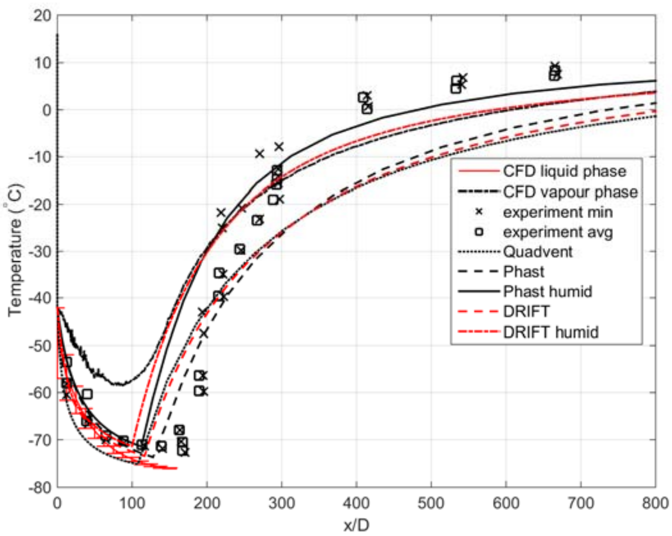

Figure 1: Liquid and vapour phase CFD results for mesh 6 (20 μm droplets) plotted alongside the experimental results and the integral model results. The error bars on the liquid temperatures represent the maximum and minimum droplet temperatures at each location

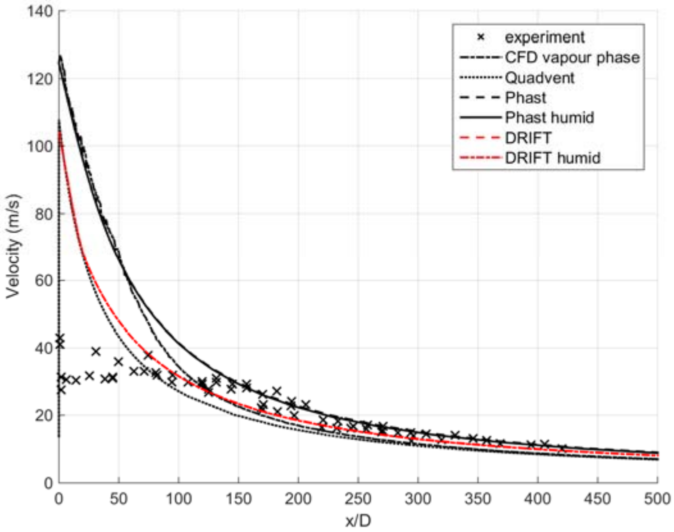

Figure 2: CFD vapour phase centreline velocity for mesh 6 plotted against the experimental values and the integral model results (the DRIFT 3 and Phast plots with and without humidity are overlaid)

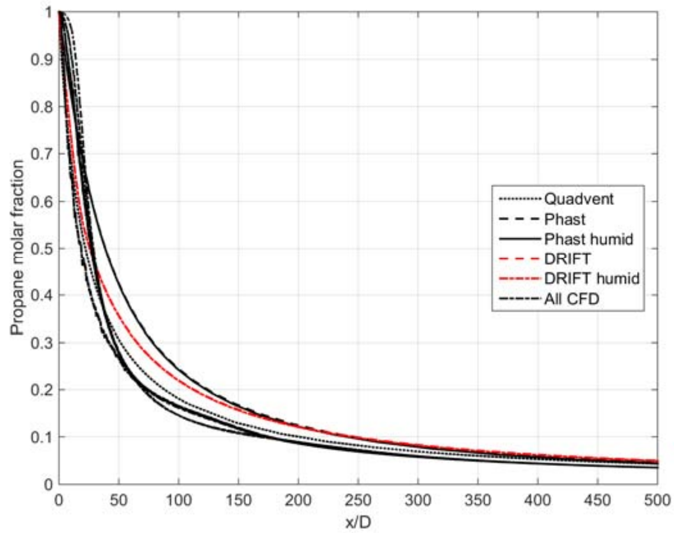

Figure 3: Model concentration predictions for all CFD runs and integral models (the DRIFT 3 and Phast plots with and without humidity are overlaid)

5. Conclusions

Small-scale flashing propane jets have been simulated using three different integral models and a CFD model. The integral models all assumed homogeneous equilibrium between the droplets and the vapour phase whereas the CFD model used a particle-tracking approach which explicitly modelled the heat and mass transfer between phases. Source conditions for the CFD model were provided by the discharge and expansion model in DNV Phast. Two sets of model predictions were obtained from the DRIFT 3 and Phast integral models, both with and without humidity effects.

The results showed that the assumption of homogeneous equilibrium in the three integral models provided a generally good approximation to the measured temperature and velocity profiles, other than the velocity close to the source. The model predictions that accounted for humidity effects gave best agreement with measured temperatures. The CFD model slightly underpredicted the vapour-phase temperatures in the far-field, which may be due in part to humidity effects not being accounted for in the CFD model. In the near-field, the CFD results showed that the vapour temperatures were not in equilibrium with the liquid temperatures, even using the smallest droplet size tested (20 µm). All of the models produced similar concentrations in the far-field at a distance of 500 orifice diameters, where the propane concentration was around 0.05 mol/mol.

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Disclaimer

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References

Allen, J. T., (1995), “Conventional temperature measurements in small scale two-phase flashing propane jet releases,” HSL report IR/L/FR95/5.

ANSYS (2013) ANSYS CFX-15 User Guide, ANSYS, Inc., Canonsburg, Pennsylvania, USA.

Bricard, P, and Friedel, L., (1998) “Two-phase jet dispersion,” Journal of Hazardous Materials, Vol 59, pp 287-310.

Britter, R., Weil, J., Leung J. C. and Hanna, S., (2011), “Toxic industrial chemical (TIC) source emissions modeling for pressurized liquefied gases,” Atmospheric Environment, 45 pp 1-25.

Dixon, C. M., Gant, S. E., Obiorah, C. and Bilio, M., (2012), “Validation of Dispersion Models for High Pressure Carbon Dioxide Releases,” IChemE symposium series No. 158, (Hazards XXIII), November 2012, Southport, UK.

DNV, (2011), “Phast release notes for V6.7,” DNV Software, London.

Fletcher, B., (1984), “Flashing flow through orifices and pipes,” Chemical Engineering Progress,” 80(3), pp 76-81.

Kelsey, A., (2001), “CFD modelling of flashing jets: Simulation of flashing propane jets,” HSL report CM/00/02.

Kelsey, A. and Ivings, M. J., (2010), “Indoor area classification calculations in support of EI15,” HSL report MSU/2010/19.

Menter, F. R., (1994) “Two-equation eddy-viscosity turbulence models for engineering applications,” AIAA J. 32, 1598-1605.

Polanco, G., Holdø, A. E. and Munday, G., (2010), “General review of flashing jet studies,” Journal of Hazardous Materials, Vol 173, Issues 1-3, pp 2-18.

Reitz R.D. and Diwakar, R., (1987), “Structure of High-Pressure Fuel Sprays,” SAE Technical Paper, 870598.

Richardson, S. M., Saville, G., Fisher, S. A., Meredith, A. J. and Dix, M. J., (2006) “Experimental determination of two-phase flow rates of hydrocarbons through restrictions,” Process Safety and Environmental Protection, 84(B1), pp 40-53.

Tickle, G. A., (1997), “EJECT - an integral model of an elevated two-phase jet in a cross-flow: theory manual for EJECT version 1.00,” AEA Technology report AEAT-1517, issue 1.

Tickle, G. A. and Carlisle, J. E., (2008), “Extension of the dense gas dispersion model DRIFT to include buoyant lift-off and buoyant rise,” Health and Safety Executive research report RR629.

Tickle, G. A., Jones, S. J., Martin, D., Ramsdale, S. A. and Webber, D. M., (1997), “Development and Validation of Integral Models of Two-Phase Jets,” AEA Technology report AEAT/1389, Issue 1

Webber D. M., Ivings M. J. and Santon R. C., (2011), “Ventilation theory and dispersion modelling applied to hazardous area classification,” Journal of Loss Prevention in the Process Industries, volume 24, issue 5, pp 612-621.

Wheatley, C.J., (1987), “Discharge of liquid ammonia to moist atmospheres - survey of experimental data and model for estimating initial conditions for dispersion calculations,” SRD, report SRD/HSE/R410.