CFD Design Model for Sparkling Diminutive Propane Jet

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ABSTRACT

Accidental releases of pressure liquefied materials can result in sparkling, vaporizing jets that mix with ambient air and disperse. It's critical to accurately characterize the early jet behavior in consequence modeling because it can affect the subsequent vapour dispersion. For modeling sparkling jets and their dispersion, a variety of approaches are available, with Computational Fluid Dynamics (CFD) becoming increasingly popular. By comparing model predictions to experimental data and other models, one can build confidence in their accuracy. The CFD modeling of a small-scale flashing propane jet is described in this study, along with comparisons to actual data and integral model predictions.

Keywords: *Sparkling, Propane jets, Model, CFD*

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1. INTRODUCTION

Sparkling jet models are frequently used to give the input, or source term, for vapour dispersion calculations for examining the repercussions of a discharge of a pressurized liquefied gas. That is, the initial discharge, rapid expansion, mixing, and vaporization are all included in the sparkling jet model. The result of these computations is the source term, which can be fed into an atmospheric dispersion model, which defines the gas cloud's subsequent dispersion. Using the initial storage conditions, leak dimensions, and material parameters, the sparkling jet model estimates a source term that typically includes temperature, velocity, concentration, and liquid fraction.

Modeling of sparkling jets is frequently broken down into many steps. First, determine the discharge conditions at the pipe or vessel's exit; second, describe the initial liquid expansion to atmospheric pressure; and third, determine the dispersion of the two-phase mixture into air, where the droplets evaporate into vapour. These stages are chosen as much for modeling convenience as for physical reasons, even though they are meant to represent observed behavior. There have been a variety of flashing jet models produced, ranging from simple expressions to integral (whole jet) models to Computational Fluid Dynamics (CFD) simulations. Each approach has advantages and disadvantages, and the robustness of each model must be thoroughly tested (validated) using experimental data.

2. SMALL SCALE SPARKLING EXPERIMENTS

Tests on sparkling releases have been conducted in a variety of ways, with the most common being dispersion experiments (both laboratory and field size) and discharge experiments. Bricard and Friedel (1998) give an overview of dispersion experiments as well as the various modeling approaches that were available at the time. Many discharge experiments have been conducted in the past to determine flow rates from pipes, orifices, and tubes in order to provide data for pressure relief and venting system models, as well as to determine source terms for dispersion modeling. Fletcher (1984) and Richardson et al. (2006) provide examples of discharge experiments, and Polanco et al. (2006) provide an overview of experimental data (2010). Measurements were mostly concerned with the discharge rate or far-field dispersion in many research available in the public domain, and only a few sought to study the parameters of the jet near the exit. This is presumably owing to the difficulties of taking reliable measurements in a flashing two-phase flow.

Allen (1995) conducted studies on propane releases at saturation circumstances through 4 mm diameter, 40 mm length pipes in small scale observations in flashing jets. Thermocouples were initially used to measure temperature, but the measurement program was later expanded to incorporate velocities. Table 1 lists the details of the trials, which were gleaned from Allen (1995)'s data report and Tickle et alreport .'s on one-dimensional modeling (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)	84.7

3. LASHING JET MODELS

Many models exist for calculating flashing release danger ranges, although calculation approaches that produce 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 for a given orifice size. Wheatley (1987) offers a model for calculating jet parameters from ammonia flash discharges, which includes the thermodynamics of mixing ammonia with atmospheric moisture. Tickle's (1997) EJECT model for flashing jets was later incorporated into Tickle and Carlisle's (Tickle and Carlisle, 2008) DRIFT 3 gas dispersion model. The dispersal stage of flashing jets has been successfully simulated using computational fluid dynamics (Kelsey, 2001; Dixon et al., 2012); however, in both cases, the simulations began after the flashing depressurisation region, and an additional model was used to perform the initial flashing calculations. Britter et al. (2011) provide a review of flashing release modeling methodologies, encompassing both pure liquid and two-phase discharge from various sources such as pipelines, tubes, and fissures. The ambiguity surrounding the conditions at the exit is one of the key challenges in modeling orifice type flashing flows, and many experimental studies could not capture the flow detail in this region.

Three different integral models were examined in this study: DRIFT 3.7.2, Phast 6.7, and QUADVENT 1.9.9.17. In the 1990s, ESR Technology created the DRIFT (Dispersion of Releases Involving Flammables or Toxics) model for the UK Health and Safety Executive (HSE), which was recently updated to DRIFT 3. DRIFT 3 includes a jet model to anticipate dispersion from pressurised releases, and it can represent ground-based or elevated clouds that are released either instantly or as a steady continuous source. DNV Phast (DNV, 2011) is a general-purpose consequence modeling tool that includes models for depressurization, flashing, and dispersion. The Health and Safety Laboratory developed QUADVENT (Webber et al., 2011) as a tool for conducting area classification investigations (HSL). It was originally designed to simulate gas jets, but it was recently altered to simulate flashing liquid releases. The capacity of QUADVENT to predict interior releases in the absence of wind and to account for the accumulation of gas in an enclosed environment distinguishes it from other dispersion models. DRIFT 3 and Phast were used to run simulations with and without humidity effects.

4. CFD MODELLING

From the point at which the jet has grown to atmospheric pressure, the general-purpose CFD code ANSYS CFX 15 (ANSYS, 2013) was used to model it. Because detailed modeling of the initial discharge and flashing process is not commonly done with CFD in consequence modeling applications, it was not tried. For non-flashing jets, determining the break-up of a liquid stream into droplets is exceedingly difficult, and the models designed for this purpose are often focused at the type of flow encountered in automotive fuel injection systems. As a result, DNV Phast was utilized to represent the initial expansion process, with the post-expansion circumstances being fed into the CFD model as shown in Table 2. The spray of liquid droplets, their subsequent evaporation, and the diffusion of vapour in the jet were all modeled using CFD. The CFD model employed an Eulerian-Lagrangian technique to do this, in which the vapour flows through a fixed computational mesh in space. The velocity, temperature, pressure, and concentration distributions are determined by solving the momentum, mass, and energy conservation equations in each mesh cell. The droplet spray was modeled using Lagrangian particle tracking. Discrete computational particle motions are tracked from their injection point through the flow domain until they collide with a solid surface, leave the domain, or completely evaporate.

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

A 2 m diameter by 4 m long cylinder with a cylindrical pipe section equal to the enlarged diameter projecting 40 mm from one of the round end faces formed the domain. Tetrahedral cells were used to mesh the domain, and a near-wall inflating layer of prismatic cells was applied to the pipe surfaces. Six meshes with 0.1 to 4.2 million nodes each were constructed and refined in the region of the jet.

4.2 Input parameters

The CFD model was run with the following input parameters:

- Phase liquid With a co-flow of vapour, Lagrangian particles were injected at the pipe's end.
- Set the domain's ends and sides to be openings with no 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
- Vapour phase turbulence is controlled by the inlet velocity and 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) shows the temperature data as a minimum temperature as well as an average over a long period of time. Because the temperature data were taken using bare thermocouples, a flashing two-phase jet may reflect a mix of diverse physical processes. Liquid droplets could collide with the thermocouple, causing it to evaporate and indicate a low temperature, or water condensed from the environment could form an ice layer. Furthermore, measurements taken by arresting a high-speed flow will tend to be slightly higher than non-invasive observations, but this effect is likely to be minor (on the scale of a few K) for the flows in question. As a result, the temperature data will be a mass average of the continuous and liquid phases. Two temperatures were recovered for the CFX results: the centreline vapour phase temperature on the Eulerian mesh and the liquid temperature. The latter was calculated by averaging particle temperatures along the jet's centerline.

4.4 Results

The overall temperature forecasts are compared to the measured readings from Allen in Figure 1. (1995). Temperatures are displayed versus downstream distance, x, and nozzle diameter, D, normalized. The first flashing expanding region is assumed to be a short distance in all models, and the results are displayed from the point where atmospheric pressure is attained and the liquid reaches its boiling point. The CFD results were obtained using the least "cost" simulation — a coarse 0.1 million node mesh with 2,500 particles, 10 integration steps per element, and a particle size of 20 m. The error bars indicating the maximum, minimum, and average over all the particles at each position show the expected liquid temperatures in red. Allen's (1995) experimental measurements are presented as a minimum value and an average minimum. It is likely that measurements in the region where droplets are present are skewed towards the droplet temperature, hence it is appropriate to compare with the CFD projected liquid temperatures. The CFD results are in reasonable agreement with the trials in the liquid-filled zone on this premise. The highest temperature is somewhat overpredicted, while the lowest is slightly underpredicted. Even with the small 20 m droplets, the CFD model accurately predicts droplet persistence, but the temperature differential between liquid and vapour temperatures indicates that equilibrium is not reached. All of the models significantly underestimate the temperature rise in the region of the jet after all of the liquid has evaporated. QUADVENT, DRIFT 3, and Phast all produced similar findings in this region, however DRIFT 3 and Phast projections that included ambient humidity were more accurate due to the heat released by condensation. The CFD model with the bigger initial particle diameter shifted the liquid temperature further away from equilibrium, but had no effect on the far-field temperatures, velocity, or concentration.

The vapour phase velocities for the four models are compared to the data in Figure 2. For x/D values bigger than about 100, there is good agreement between the models and the measurements. The data up to this point indicate a discharge velocity of about one-third of that projected. This could be owing to the unpredictability of the state of the substance exiting the orifice. Two-phase flows are very compressible, and if flashing occurs in the pipe, choking at the outlet will limit the discharge velocity. The anticipated concentrations are what matter in consequence modeling, and as shown in Figure 3, all of the models produce extremely similar forecasts by x/D of 500, where the concentration is around 0.05 mol/mol. Over all of the parameter ranges investigated in the CFD model, the integral models (which all assume homogeneous equilibrium) produce identical concentrations to the CFD model.

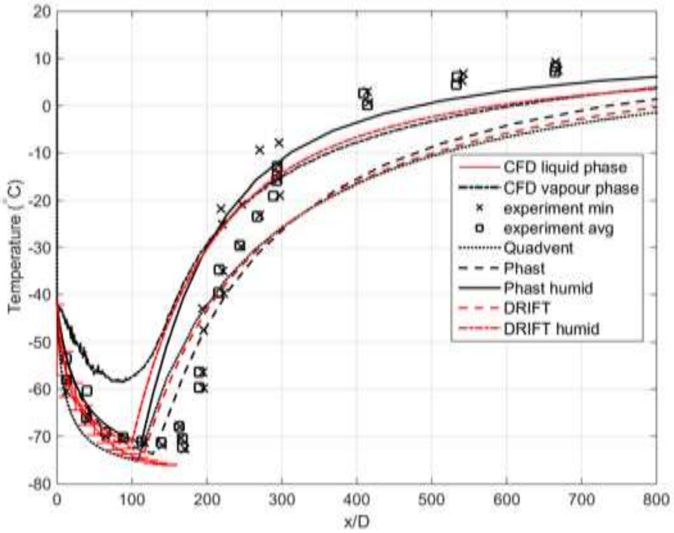

Figure 1: Liquid and vapour phase CFD results for mesh 6 (20 µm droplets) plotted alongside the experimental results and the integral model results. The error bars on the liquid temperatures represent the maximum and minimum droplet temperatures at each location

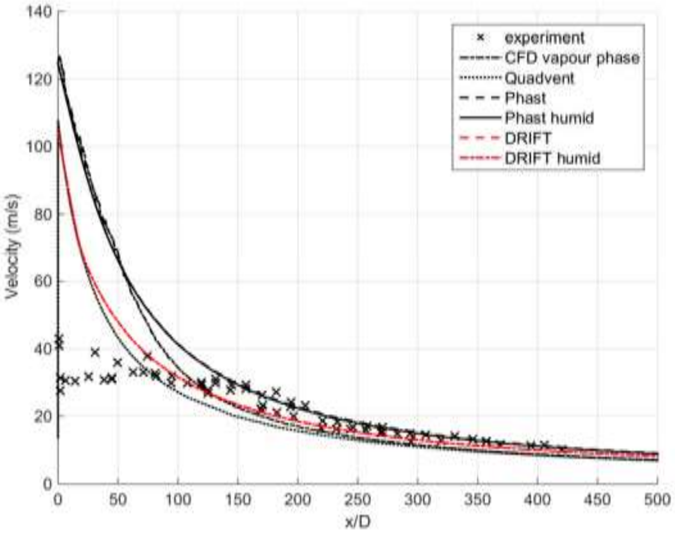

Figure 2: The actual measurements and the integral model results are displayed against the CFD vapour phase centreline velocity for mesh 6 (the DRIFT 3 and Phast plots with and without humidity are overlaid)

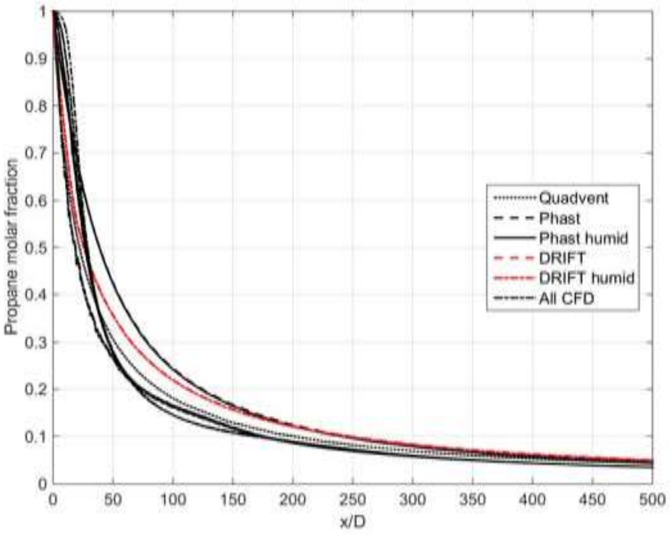

Figure 3: All CFD runs and integral models have concentration forecasts built in (the DRIFT 3 and Phast plots with and without humidity are overlaid)

5. CONCLUSIONS

Three integral models and a CFD model were used to simulate small-scale sparkling propane jets. The integral models all assumed homogenous equilibrium between the droplets and the vapour phase, but the CFD model employed a particle-tracking approach to explicitly model heat and mass transfer between the phases. The discharge and expansion model in DNV Phast provided source conditions for the CFD model. The DRIFT 3 and Phast integral models produced two sets of model predictions, one with and one without humidity effects.

The results showed that, with the exception of the velocity close to the source, the assumption of homogeneous equilibrium in the three integral models provided an excellent approximation to the actual temperature and velocity profiles. Model projections that took humidity effects into account had the best agreement with measured temperatures. The vapour-phase temperatures in the far-field were slightly underpredicted by the CFD model, which could be owing to humidity effects not being accounted for in the CFD model. Even with the smallest droplet size measured (20 m), the CFD results showed that the vapour temperatures were not in equilibrium with the liquid temperatures in the near-field. At a distance of 500 orifice diameters, all of the models produced identical propane concentrations in the far-field, which were around 0.05 mol/mol.

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