

Comparisons of the predictions of the gas dispersion model DRIFT against data for hydrogen, ammonia and carbon dioxide

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DRIFT is an integral model for predicting the dispersion of gaseous and two-phase releases in the atmosphere. DRIFT is mainly used for the purpose of assessing toxic and flammable dispersion for major hazards. This paper presents the results of new validation studies comparing DRIFT predictions with dispersion data for hydrogen, ammonia and carbon dioxide (CO₂) substances.

The hydrogen jet dispersion comparisons provide a test of the dispersion model at much higher pressure and lower molecular weight than previously.

DRIFT includes a model for the non-ideal solution of ammonia and water in the liquid aerosol phase. The comparisons against the FLADIS ammonia field experiments provide a test of DRIFT for two-phase ammonia jet releases under moist atmospheric conditions typical of the UK and Northern Europe. DRIFT's predictions of aerosol composition compare favourably with measurements. Good agreement is found with concentration measurements for which there is negligible sensitivity on whether ammonia-water interactions or an ideal solution model is used.

To enable comparisons with two-phase carbon dioxide data, it was necessary to extend DRIFT's thermodynamic modelling to include the effect of solid carbon dioxide (dry ice) aerosol. Comparisons against data released by the CO₂PIPETRANS Joint Industry Project (JIP) indicates good performance of the resulting DRIFT predictions.

The results of the comparisons of this study are encouraging and support the use of DRIFT for assessing dispersion of hydrogen, ammonia and carbon dioxide.

Keywords: Hydrogen, ammonia, carbon dioxide, dispersion modelling, model validation.

Introduction

Arising from the pressing need to tackle climate change, there is an ever-increasing focus on new decarbonisation technologies. Promising technologies include using hydrogen as a fuel, which is seen as a good way of limiting carbon dioxide emissions to the atmosphere. Binding hydrogen with nitrogen in the form of ammonia can be used for the bulk storage and transport of hydrogen. Large-scale carbon capture and storage projects may involve transport of large quantities carbon dioxide. Of key interest is the extent that established consequence assessment tools traditionally used for hydrocarbon and chemical hazards can also be applied to these new technologies.

DRIFT is an integral model for predicting the dispersion of gaseous and two-phase releases in the atmosphere. The model originates from the work of Webber et al. (1992) and has subsequently been further developed and improved to include modelling of momentum jets and buoyant dispersion, as well as allowing modelling of multi-component behaviour and the inclusion of longitudinal dispersion for finite-duration and time-varying dispersion (Tickle and Carlisle, 2008). DRIFT is mainly used for the purpose of assessing toxic and flammable dispersion for major hazards.

This paper presents new validation studies comparing DRIFT predictions with dispersion data for hydrogen, ammonia and carbon dioxide jet releases. The modelling includes the thermodynamic behaviour of liquid ammonia aerosol (ammonia in solution with condensed water vapour) and two-phase carbon dioxide (solid and vapour) jets.

Hydrogen jet data

Papanikolaou and Baraldi (2011) compared Computational Fluid Dynamic (CFD) model predictions for concentration and axial velocity against measurements from experiments involving hydrogen jet releases from high pressure storage. Gas releases from high pressure are characterised by the formation of shock structures near the release point and are classified as being "under-expanded", meaning there is a rapid expansion phase prior to achieving behaviour resembling that of an isobaric sub-sonic jet. Rather than modelling the jet shock structure, many dispersion models adopt simpler pseudo-source models for this region. For under-expanded gas jets, DRIFT adopts the pseudo-source method of Birch et al. (1987) – this approach was originally validated against observations of high pressure (up to ~70 bar) methane jets.

Table 1 summarises the release conditions taken from Papanikolaou and Baraldi (2011)

Table 1 - Hydrogen jet release conditions

Parameter	Value
Substance	Hydrogen
Pressure	98.1 bara
Temperature	14.5°C
Nozzle Diameter	1 mm
Release Orientation	Horizontal
Release Height	0.9 m
Discharge Coefficient	0.91
Discharge Rate	0.0044 kg/s

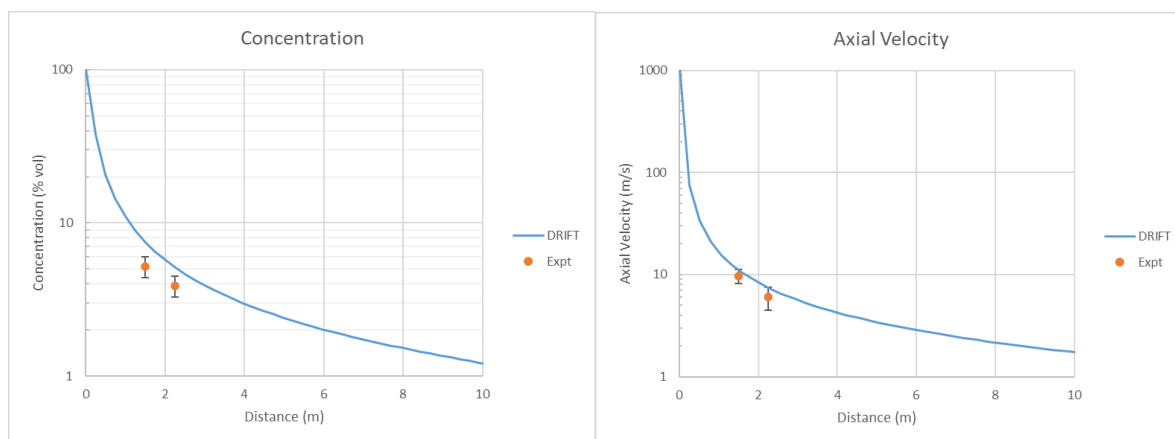


Figure 1 - DRIFT predictions of hydrogen concentration and axial velocity along the jet centreline.

Figure 1 shows DRIFT’s predicted axial velocity and concentration along the centreline of the jet as a function of axial distance. The data points are the mean experimental values extracted from Figures 3-6 of Papanikolaou and Baraldi (2011). The error bars of the data points correspond to +/-1 standard deviation of the experimental values.

DRIFT’s predictions are slightly higher than the measured values, with the closest agreement for velocity. The DRIFT predictions for velocity are within +1 standard deviation of the measurements and for concentration are within +50% of the measurements. The closer agreement for velocity than concentration implies that there might be scope for slightly improving DRIFT’s predictions by allowing for different spreading rates of scalar quantities (mass, species) and vector quantities (momentum) in the jet. Some jet models include such empirical factors, however making such a change to DRIFT would require care to ensure that this does not impair agreement for other jet regimes such as those involving dense two-phase jets.

Given the high pressure of the release, the low molecular weight for hydrogen and the fact that there has been no specific tuning of the model to hydrogen releases, the overall level of agreement with measurements is judged as being acceptable.

Ammonia field trials

In the FLADIS ammonia field trials, superheated anhydrous liquid ammonia was discharged through a nozzle (Neilsen and Ott, 1996; Neilsen et al. 1997). The experiments were undertaken at a test site in Landskrona, Sweden. Figure 2 shows the release system used in the experiments.

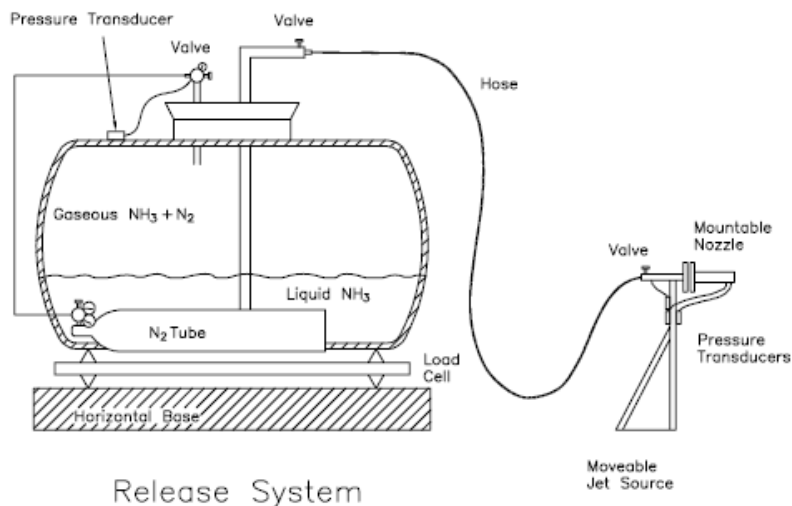


Figure 2 - The release system in the FLADIS field experiments (Neilsen and Ott, 1996).

The release and ambient conditions of the trials are summarised in Table 2. Only those trials for which Neilsen and Ott (1996) present concentration measurements are included. Concentration measurements were made using sensors on arcs at downwind distances of approximately 20 m, 70 m and 240 m; in some trials measurements are only available at 20 m and 70 m. Neilsen and Ott (1996) present centreline concentrations analysed using two approaches:

1. Fixed frame analysis. This is the traditional analysis which fits Gaussian profiles to the measurements averaged over the duration of observation. The effects of lateral meander of the plume centre due to changing wind direction leads to a wider time-averaged cloud and a reduction in the time-averaged centreline concentration.

2. Moving frame analysis. This analysis fits a Gaussian horizontal profile to the instantaneous plume centroid position at each time – this effectively removes the effect of lateral meander due to changing wind direction – this results in higher centreline concentrations and a narrower cloud. The advantage of the moving frame analysis is that it is less prone to changing wind direction during the trial (e.g. as happened for trial 9). Also, this analysis is more suitable for comparing with models that do not account for the effect of changing wind direction, e.g. wind tunnel studies, or short time averaged integral model predictions.

Table 2 - Experimental conditions for FLADIS ammonia field trials (Nielsen and Ott, 1996)

Trial	Ø (mm)	Angle	P ₀ (bara)	T ₀ (°C)	\dot{m} (kg/s)	T _{dur} (min)	u ₁₀ (m/s)	u* (m/s)	L (m)	P _{air} (mbar)	T _{air} (°C)	r.h. (%)
9	6.3	→	6.9	14	0.40	15	6.1	0.44	348	1020	16	86
12	4.0	↑	7.2	16	0.20	5	2.2	0.15	-61	999	16	75
13	6.3	→	7.7	18	0.50	15	5.5	0.48	-164	1008	16	52
14	6.3	→	7.4	17	0.47	10	5.2	0.45	-174	1008	17	53
15	6.3	→	7.7	18	0.51	3	5.9	0.50	271	1019	17	60
16	4.0	→	8.0	17	0.27	20	4.4	0.41	138	1020	16	62
17	4.0	→	7.9	15	0.27	25	3.7	0.31	59	1020	16	63
20	4.0	→	7.9	16	0.23	40	4.0	0.38	-25	1018	20	69
21	6.3	→	6.5	12	0.57	40	4.3	0.34	-53	1017	21	59
23	6.3	→	7.6	16	0.43	20	6.6	0.53	-112	1012	17	54
24	6.3	→	5.7	9	0.46	10	4.9	0.41	-77	1013	18	54
25	6.3	→	5.9	9	0.46	22	4.5	0.43	-201	1013	17	54
26	4.0	→	8.3	20	0.21	10	3.0	0.29	-16	1019	19	52
27	4.0	→	8.5	20	0.22	21	2.4	0.25	-22	1019	19	50

Ø: nozzle diameter; →: horizontal release; ↑: vertical release; P₀: exit pressure; T₀: exit temperature; \dot{m} : discharge rate; T_{dur}: release duration; u₁₀: windspeed at 10m height; u*: friction velocity; L: Monin-Obukhov length; P_{air}: air pressure; T_{air}: air temperature; r.h.: relative humidity.

Note: Exit pressure and temperature measured a short distance upstream of the open end of the discharge nozzle.

DRIFT includes a thermodynamic model (Wheatley, 1987) for the non-ideal solution of ammonia and water in the liquid aerosol phase. The effect of the non-ideality is that ammonia can persist longer in solution with condensed water vapour than for an ideal solution, or for a water immiscible substance. Another effect is that the heat of solution of ammonia and water is added to the cloud which can reduce dense gas effects and, in some circumstances, this may lead to buoyant behaviour. The base case runs for comparison with the FLADIS field trials data are using the non-ideal ammonia water solution model. Sensitivity runs have also been performed assuming an ideal solution neglecting the interactions between ammonia and water.

DRIFT runs have been undertaken for all the FLADIS field trials listed in Table 2. Following Nielsen and Ott (1996), a roughness length of 0.04 m has been used. To minimise the effect of the wind direction changing during the trials, this paper presents comparisons of the moving frame concentration results with DRIFT's short time average predictions. As an example, Figure 3 shows centreline concentration comparisons for four representative trials. The DRIFT results in Figure 3 have been extracted at heights that match the sensor heights which reported the maximum concentrations at each distance. An exception is trial 12 which is a vertical release – in this case DRIFT predicted that the jet is still elevated at 20 m distance resulting in zero concentration prediction at the nearest sensor location, the comparison shown for trial 12 at this distance is with DRIFT's elevated centreline concentration.

Figure 4 shows a plot of the geometric variance $VG = \exp\left\{\left[\log_e\left(\frac{C_m}{C_p}\right)\right]^2\right\}$ and geometric mean bias $MG = \exp\left(\log_e\left(\frac{C_m}{C_p}\right)\right)$ for the ratio of the measured, C_m, to predicted, C_p, centreline concentrations for all the FLADIS trials in Table 2. The measured values are from the moving frame analysis and the predicted are using DRIFT's short time averaging option. In this plot, perfect agreement all the time would give rise to VG = MG = 1. The DRIFT predictions show a small overprediction and variance - these values are well within acceptable ranges typically adopted by model evaluation studies (see e.g. Ivings et al, 2007 for LNG).

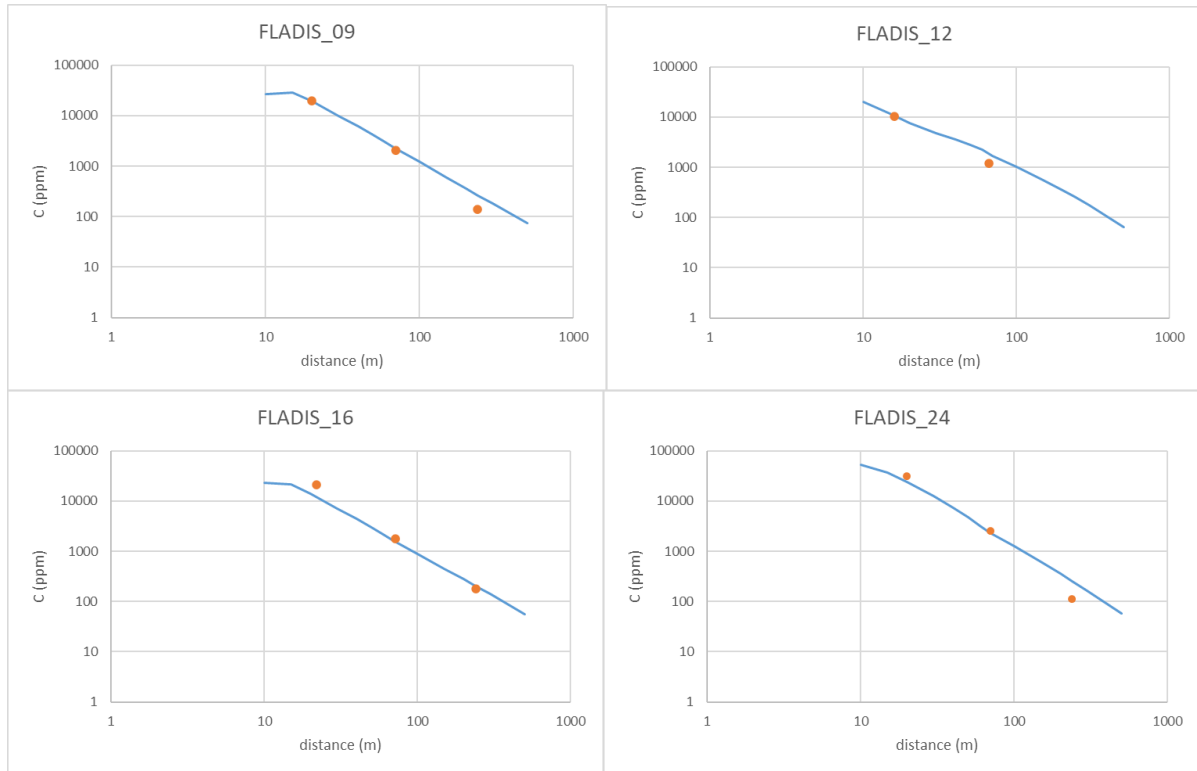


Figure 3 – DRIFT predictions of centreline concentrations for FLADIS trials 9, 12, 16 and 24. Dots are measurements, line is model prediction

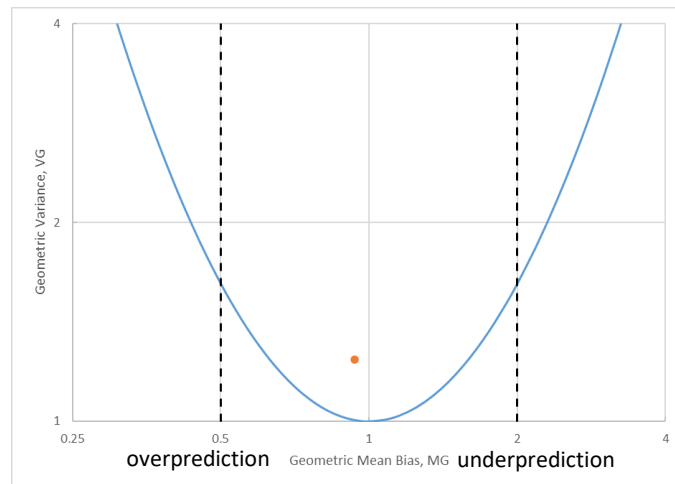


Figure 4 – Plot of geometric mean bias and geometric variance for measured to predicted centreline concentrations from the FLADIS ammonia field trials. The dashed vertical lines at $MG = 0.5$ and $MG = 2$ represent a factor of two overprediction and factor of two underprediction about the mean. The parabolic line represents the minimum possible VG for a given MG. The dot represents the model performance.

Figure 5(a) compares the measured composition of liquid samples collected between 4 m and 12 m downstream from the source with DRIFT predictions. Both the measured samples and DRIFT predictions show the composition changing within a few metres from almost pure ammonia to almost pure water. There is good agreement between the model and the measurements at 4 m, after which DRIFT predicts a more rapid decrease in ammonia content, approaching the measured values again near 12 m. Figure 5(b) shows the effect of assuming an ideal solution (Raoult's Law) for the ammonia-water system – the results are similar to the non-ideal case (the default in DRIFT) at 4 m, but the ammonia is less persistent in the ideal solution giving lower ammonia content than observed at 12 m. There is however negligible effect on the VG and MG for the concentration predictions, which if plotted in Figure 4 would give a point coincident with the dot for the default (non-ideal solution) case. This indicates that, for the FLADIS field trials, the non-ideal thermodynamic behaviour evident in the measured compositions at short distances is having negligible impact on the predicted, and given the close agreement presumably also the measured, concentrations at greater distances.

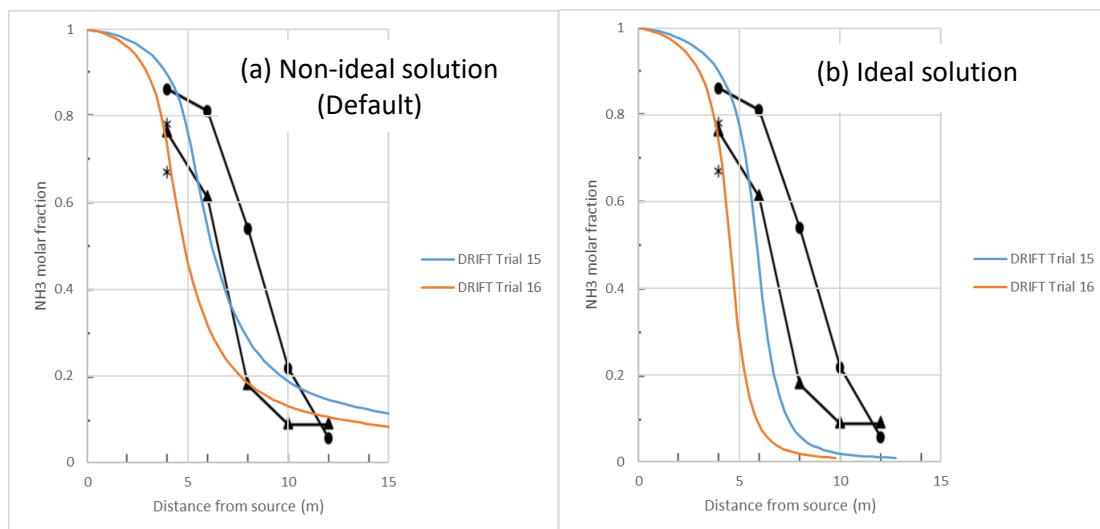


Figure 5 – Composition of liquid samples in FLADIS trial 15 (dots are measured values) and trial 16 (triangles are measured values) compared with DRIFT predictions as a function of distance from the source. The two ice samples (* symbols) are taken from trial 16 and 17 which both had release rates of 0.27 kg/s. (a) DRIFT results assuming non-ideal solution of ammonia with water (the default), (b) Sensitivity assuming ideal solution of ammonia with water.

Carbon dioxide field trials

Figure 6 shows a schematic of the phase diagram for CO₂. Releases from pressure liquefied CO₂ conditions are likely to result in a two-phase jet consisting of solid CO₂ (dry ice) and CO₂ vapour at atmospheric pressure. The dry ice will sublime as the jet entrains air, lowering the temperature of the jet due to the heat of sublimation. After the dry ice has all sublimed the CO₂ disperses as a cold vapour jet, possibly with condensed water from the atmosphere.

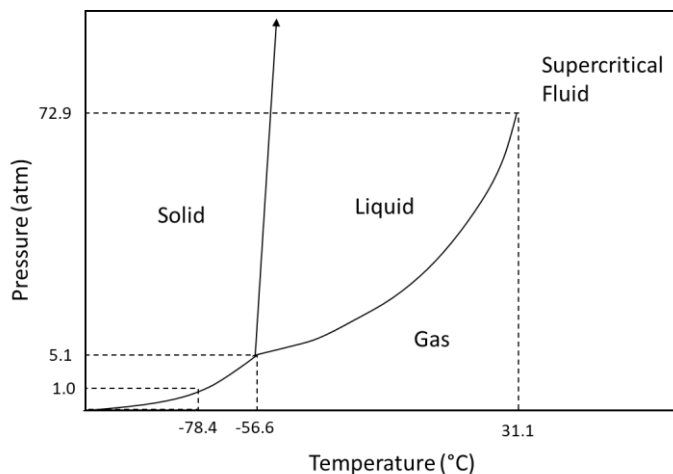


Figure 6 - CO₂ phase diagram (schematic).

To enable comparisons with two-phase carbon dioxide data, DRIFT's thermodynamic modelling has been extended to include the effect of solid CO₂ as aerosol. This was done by following the approach of Witlox, Harper and Oke (2009) and of Webber (2011) where below the triple point the saturated liquid vapour pressure curve is replaced by the solid sublimation-vapour pressure curve and uses the heat of sublimation of the solid instead of the heat of vaporisation of the liquid. DRIFT further assumes that the two-phase flow is in homogenous equilibrium and neglects any deposition of solid CO₂ - this has been shown to be a valid approximation for free, unimpeded jets (Gant et al 2014).

As part of the CO₂PIPETRANS JIP, DNV released experimental datasets from CO₂ field trails (DNV CO₂PIPETRANS JIP data). The datasets include dataset 1 (BP data), dataset 2 (Shell data), dataset 3 (depressurisation tests on a CO₂ pipeline) and dataset 4 (experimental discharge data for large diameter CO₂ releases). For this study, comparisons are made against a subset of dataset 1 (BP data). This subset consists of horizontal non-impinging jets that are suitable for validating DRIFT's dispersion modelling. An analysis of this subset by Witlox (2012) includes DNV's ATEX model predictions of the source area immediately after expansion to atmospheric pressure that are suitable for direct input to DRIFT. Table 3 summarises the experimental conditions for the selected tests. For the steady-state tests (1, 2, 3, 5, 6 and 11) the mean values of

temperature and pressure during the discharge are used, whereas for the transient tests (8, 8R and 9) the initial values averaged over the first 20 s of the release are used.

Table 3 - Experimental conditions for BP CO₂ tests (Witlox, 2012)

	Test 1	Test 2	Test 3	Test 5	Test 6	Test 11	Test 8	Test 8R	Test 9
Discharge data									
storage phase	liquid	liquid	liquid	liquid	liquid	liquid	vapour	vapour	vapour
storage pressure (barg)	103.4	155.5	135.5	157.68	156.7	82.03	157.76	148.7	154.16
storage temperature (°C)	5	7.84	11.02	9.12	9.48	17.44	147.12	149.37	69.17
vessel volume (m ³)	-	-	-	-	-	-	6.3	6.3	6.3
orifice diameter (mm)	11.94	11.94	11.94	25.62	6.46	11.94	11.94	11.94	11.94
discharge rate (kg/s)	8.2	11.4	9.9	40.7	3.5	7.1	3.39	3.0	4.49
discharge duration (s)	60	59	60	40	120	58	120	132	179
Ambient data									
temperature (°C)	14.2	7.5	10.6	5.8	6.1	11.6	11.19	11.1	8.2
relative humidity (%)	74.4	96	95.8	96.7	100	94	100	100	99.9
wind speed (m/s)	4	3.44	3.37	5.13	2.20	5.99	4.71	0.76	4.04
Expanded source conditions									
temperature (K)	194.6	194.6	194.6	194.6	194.6	194.6	198.2	204.8	194.6
solid mass fraction	0.397	0.403	0.384	0.399	0.397	0.330	0	0	0.154
expanded diameter (m)	0.125	0.129	0.127	0.273	0.070	0.121	0.066	0.065	0.098

Note 1: All releases at 1.1m above ground

Note 2: Wind speed at 1.65m above pad of test rig

Note 3: Expanded source conditions from DNV ATEX model, except for temperature of solid-vapour cases which are set at the saturation temperature in DRIFT at a fixed ambient pressure of 101325 Pa.

Following Witlox (2012), an atmospheric surface roughness length of 0.1 m and neutral atmospheric stability has been assumed for the DRIFT dispersion runs.

Figure 7 and Figure 8 show the predicted CO₂ solid mass fraction and centreline temperature as functions of downwind distance from the release. The solid CO₂ is predicted to sublime over a distance of less than 10 m. The temperature profiles show a minimum in temperature when all the solid CO₂ has sublimed.

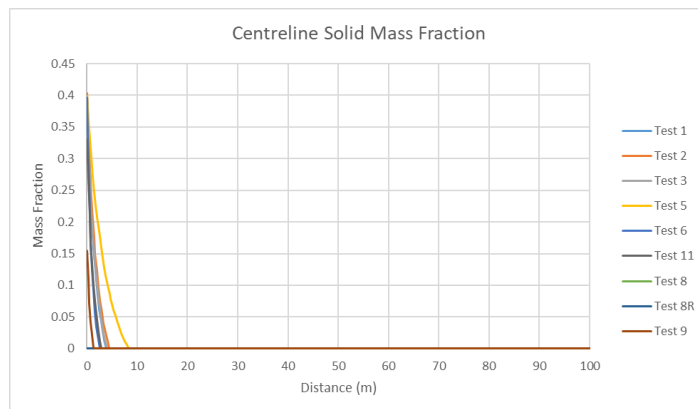


Figure 7 - DRIFT predictions of centreline solid CO₂ mass fraction for BP CO₂ tests

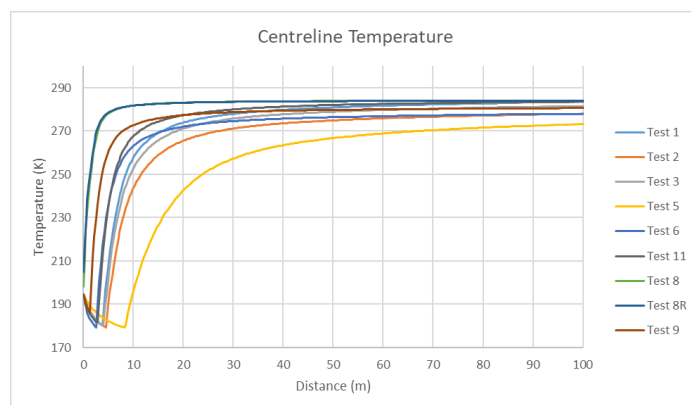


Figure 8 - DRIFT predictions of centreline cloud temperature for BP CO₂ tests.

Figure 9 show DRIFT’s predictions of centreline temperature compared with temperature measurements at various downstream distances from the pipe exit. For the purpose of this comparison, the minimum temperature at each distance (with no time averaging above the response time of the sensors) is compared with the predictions. Although the measured data points are quite scattered, for those tests predicted to have a solid fraction after flashing to atmospheric pressure, there is depression below the sublimation temperature of approximately 194K for both the measurements and predictions. Generally, the predictions reach a lower minimum temperature than observed and show a sharp rise after the temperature minimum – this minimum corresponding to the point where all the solid is predicted to have sublimated. For tests 2, 5 and 11 and to a lesser extent test 9, the measured temperature rises sooner than predicted by DRIFT. For tests 8 and 8R, which are predicted to be all vapour after expansion to atmospheric pressure, the temperature at the closest and furthest measured distance is quite well represented by the prediction, but the measurements between these are lower than predicted. Temperature measurements in this environment are challenging and at such close distances, measurements will be very sensitive to even a small spatial offset or fluctuation in the cloud. Hence, it is possible that what is being measured is more broadly representative of a spatially averaged region of the DRIFT predictions, rather than specifically the exact centreline. Bearing this is mind, we regard the observed level of agreement between the model and measurements as being acceptable for a model primarily aimed at greater distances downstream.

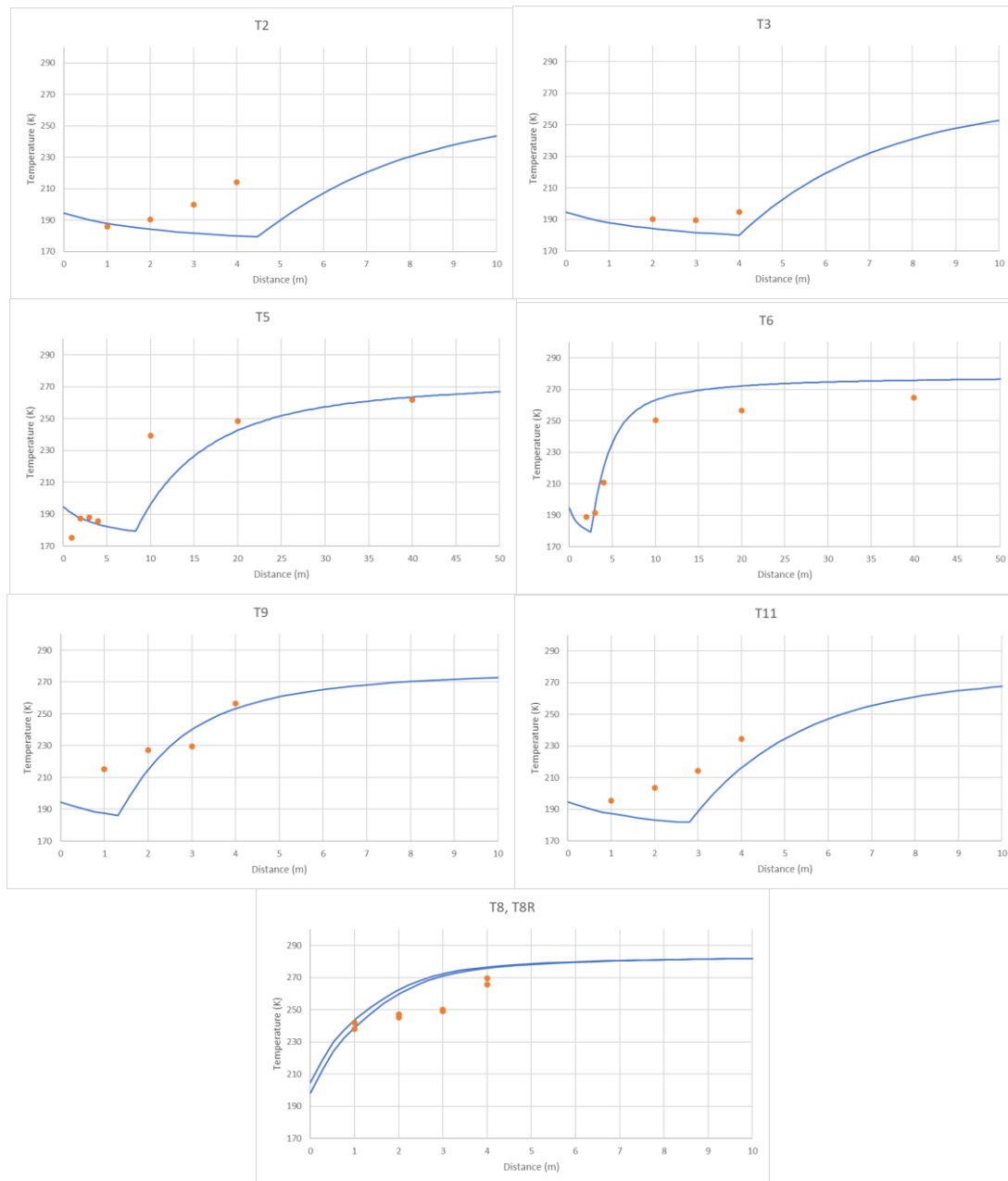


Figure 9 – DRIFT predictions of centreline cloud temperature for BP CO₂ tests compared with measured temperatures.

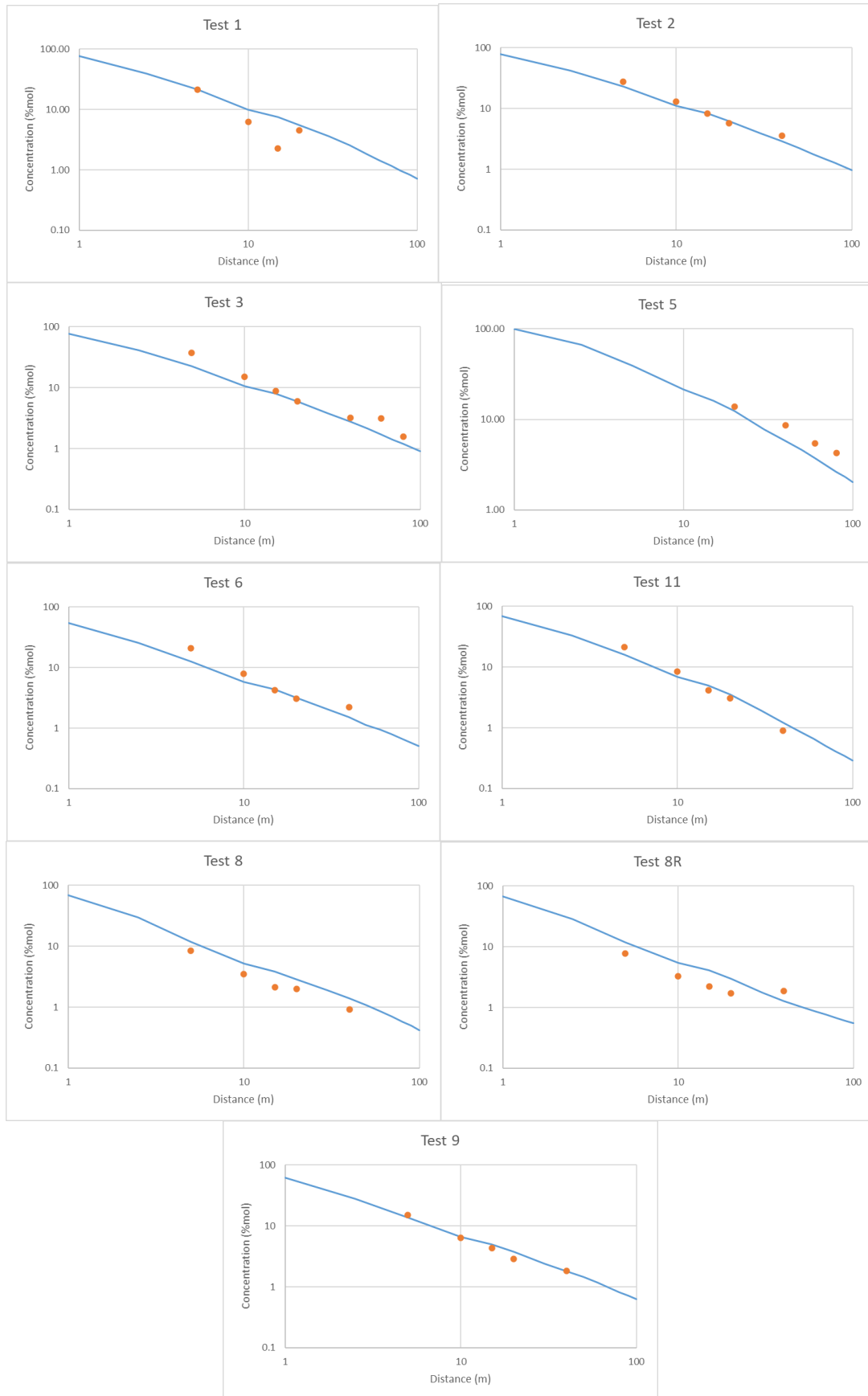


Figure 10 - DRIFT predictions of centreline concentration for BP CO₂ tests. Dots are measurements, line is model prediction

Witlox (2012) provides maximum concentration from the CO₂ tests based upon an 11-second averaging time. This averaging time was selected due to minimise the effect of changes in wind direction. Figure 10 shows DRIFT predictions of centreline concentration as functions of downwind distance compared with the 11-second averaged maxima at the worst-case (highest concentration) sensor heights. In general, there is excellent agreement between DRIFT's predictions and these measured values. A plot of the geometric variance (VG) and geometric mean bias (MG) for these data is shown in Figure 11 - this confirms the good agreement with low mean bias and low geometric variance values which are well within the acceptable range typically adopted by model evaluation studies (see e.g. Ivings et al, 2007 for LNG).

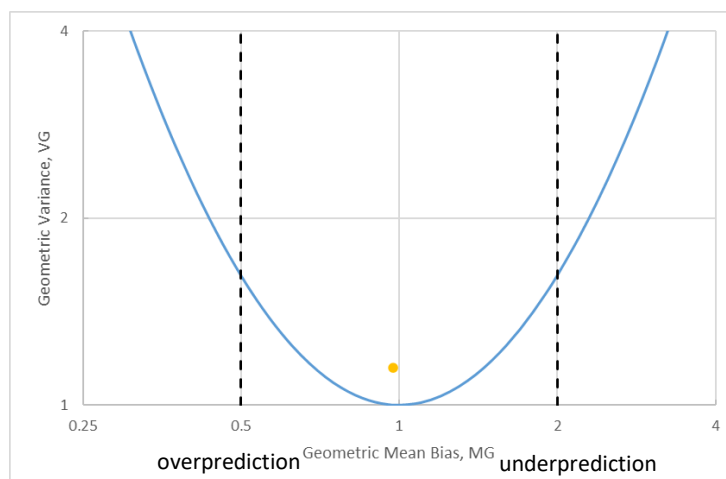


Figure 11 – Plot of geometric mean bias and geometric variance for measured to predicted centreline concentrations from the BP CO₂ tests. The dashed vertical lines at MG =0.5 and MG =2 represent a factor of two overprediction and factor of two underprediction about the mean. The parabolic line represents the minimum possible VG for a given MG.

Discussion and Conclusions

The comparisons with hydrogen data indicate slightly better agreement for velocity than concentration. It is concluded that, given the high pressure of the release, the low molecular weight for hydrogen and the fact that there has been no specific tuning of the model to hydrogen releases, the overall level of agreement for this hydrogen case is acceptable.

The comparisons with FLADIS ammonia field trial data show that DRIFT predicts a rapid change in aerosol composition near to the source, very similar to that measured. Good agreement is also found comparing DRIFT's predictions with the maximum concentrations determined from Risoe's moving frame analysis. The default in DRIFT is to include non-ideality of ammonia in solution with water and this is found to give better agreement with the measured composition of the sampled aerosol than when assuming an ideal solution with water. However, this difference does not translate to any significant impact on model performance for maximum concentrations. Whether this finding would still hold for higher release rates and lower wind speeds is something that would be interesting to investigate both theoretically using models and practically in field trials if they could be performed with larger releases under conditions of high humidity low wind speed.

To compare against the CO₂PIPETRANS carbon dioxide data, it was necessary to extend DRIFT's thermodynamics model to include sublimation of solid CO₂ – this was done following the work of Witlox, Harper and Oke (2009) and Webber (2011). Beyond this there have been no changes to the DRIFT model and no tuning for these comparisons - all the empirical parameters of the model have been left unchanged and the model inputs have been taken directly from published reports of the experiments. There are some differences in detail when comparing predictions with the temperature measurements in the very near field - given the uncertainties in the measurements, and the intended use of the model, this agreement is regarded as being acceptable. Good agreement is found between the predicted and measured concentrations, with low mean bias and variance in measured to predicted values.

The comparisons in this study have largely been based on maximum measured values compared with short time-averaged results from the model. This is useful because it is a means of dealing with the problem of wind direction changes displacing the cloud centreline during the trials. However, such wind direction changes do affect long-term predictions at a fixed point in space, for example when determining the toxic dose at a specific location. Therefore, it would be interesting to extend the analysis to also include the effect of longer time-averaging, e.g. through the use of a concentration fluctuation model for time averaging as compared with longer time averaged field data.

The datasets used in this study were selected based upon the release substance, the suitability for a paper of this length and for ease of comparison with DRIFT. Overall, the results of the comparisons in this study are encouraging and support the use of DRIFT for assessing dispersion of hydrogen, ammonia and carbon dioxide. Future studies might usefully build on this work by including model comparisons with other datasets that are available for these substances.

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