# Comparison of predictions from the gas dispersion model DRIFT (Version 3) against URAHFREP data

Graham Tickle, ESR Technology, Whittle House, Birchwood Park, Warrington, Cheshire WA3 6FW, UK

The dense gas dispersion model DRIFT has recently been extended to include the modelling of buoyant lift-off and rise. A major motivation of this extension is the modelling of hydrogen fluoride (HF) clouds in low wind, humid conditions. This paper presents comparisons of predictions using the extended DRIFT model (designated DRIFT Version 3) against data obtained from the EU URAFHREP research project. DRIFT model predictions are compared against URAHFREP wind-tunnel data for ground-level buoyant plume and puff sources. Comparisons are also made against URAHFREP field trials data for HF releases. Checks of DRIFT's HF thermodynamic model predictions against experimental data and previous model versions are included. The comparisons indicate that the extended model generally gives a good representation of the effect of buoyancy on maximum concentration and the buoyancy at which lift-off occurs. Example runs demonstrate the ability of DRIFT Version 3 to predict HF dispersion for a much wider set of atmospheric conditions than was possible with Version 2 – with a significant shortening of hazard range under conditions where buoyant lift-off is predicted.

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## Introduction

The gas dispersion model DRIFT (Dispersion of Releases Involving Flammables or Toxics) has recently been extended to include the modelling of buoyant lift-off and rise. A major motivation of this extension is improved modelling of the atmospheric dispersion of hydrogen fluoride (HF) from possible accidental releases. HF thermodynamic models suggest that, under low wind, humid conditions, initially dense HF clouds may become sufficiently buoyant for the clouds to partially or completely lift-off from the ground giving significantly reduced ground-level concentrations. HF thermodynamics and lift-off of initially ground-based buoyant clouds was studied under the EU research project URAHFREP conducted between the years 1997-2001 [3].

This paper presents comparisons of the extended DRIFT model (designated DRIFT Version 3) predictions against experimental data obtained during the URAHFREP project. The focus of these comparisons is validating and verifying[1] the URAFHREP related enhancements [1] to the DRIFT model. The comparisons cover:

- Dispersion, lift-off and rise predictions compared with wind-tunnel data for ground-level buoyant sources,
- HF thermodynamic model predictions with laboratory scale data,
- Dispersion predictions compared with URAHFREP HF field trial data,
- Comparisons with DRIFT Version 2 and sensitivity of lift-off to relative humidity.

Other comparisons of DRIFT Version 3 with DRIFT Version 2 and non-buoyant aspects are presented elsewhere [3].

## Comparisons with wind-tunnel data

As part of the URAHFREP project, BRE undertook wind-tunnel modelling on buoyant gas dispersion from ground-level sources – both steady continuous and short duration (puff) releases were modelled. Details of these wind-tunnel experiments are given in refs [5] and [6]. Data from the experiments are also included as part of the REDIPHEM database [8]. DRIFT Version 3 includes buoyant extensions based upon the recommendations in [1]. Ref [2] gives details of the mathematical model implemented in DRIFT Version 3. In the following sections we present comparisons of DRIFT Version 3 predictions with the URAHFREP wind-tunnel data for buoyant plumes [5] and buoyant puffs [6].

## Buoyant plumes

### Experimental Configuration

The buoyant plume wind-tunnel experiments [5] varied buoyancy flux, source dimensions and shape. The experimental configuration is show schematically in Figure 1. The buoyancy flux of the releases was varied whilst keeping the source momentum as low as practicable. Concentrations were measured at fixed locations on the sampling array. Following [5], all lengths are non-dimensionalised by dividing by a reference length scale, $L$ (6.7cm). The simulated rough-wall boundary layer is equivalent to an aerodynamic roughness height $z_0$ of 0.029$L$ (i.e. $z_0$/L=0.029).

[1] We distinguish between verification which involves checking that the software implementation matches the intended mathematical model equations and validation which covers determining the ability of the model equations to represent observed reality.

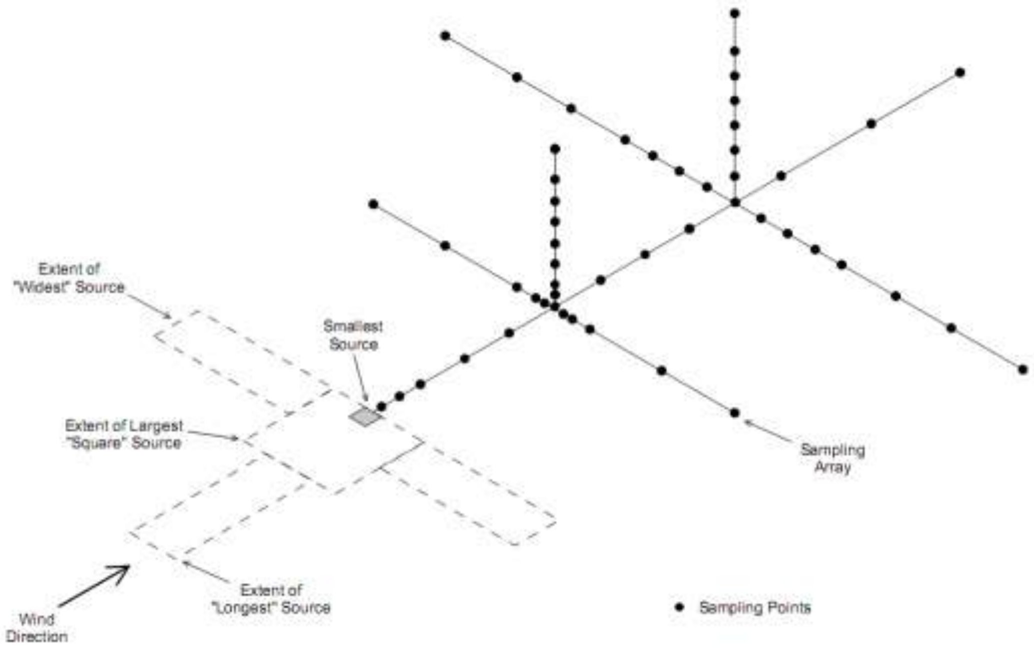


**Figure 1 Layout of concentration sampling array used in wind-tunnel experiments**

Source buoyancy for the releases is expressed via the dimensionless buoyancy flux defined as

$$\frac{F}{u^3 L} \tag{1}$$

where the (dimensional) buoyancy flux is, *F*, is:

$$F = \frac{g}{\pi} V \frac{\Delta\rho}{\rho_a} \tag{2}$$

*g* is the acceleration due to gravity

*u* is the wind speed at reference height *L*

*V* volumetric release rate from source

$\dfrac{\Delta\rho}{\rho_a} = \dfrac{\rho_a - \rho}{\rho_a}$ is the relative difference between ambient density, $\rho_a$ the source density $\rho$

The dimensionless buoyancy flux values used in the experiments and their identifying codes are shown in Table 1.

**Table 1 Dimensionless buoyancy flux values**

| *Identifying Code* | *Dimensionless Buoyancy Flux $F/u^3L$* |
|---|---|
| S | <0.001 |
| T | 0.003 |
| U | 0.01 |
| V | 0.03 |
| W | 0.1 |
| X | 0.3 |
| Y | 1.0 |
| Z | 3.0 |

## DRIFT predictions

The wind-tunnel plume releases have been modelled using DRIFT Version 3.6.15. The DRIFT modelling has been undertaken at the wind-tunnel scale. DRIFT's low momentum area source model [2] has been used for the runs. This source model permits elliptical rather than rectangular source shapes. The wind-tunnel sources have therefore been approximated by matching the source area and also matching the ratio of the downwind to cross-wind source extents.

Following [5], concentrations are presented in the dimensionless form, *K* defined by:

$$K = \frac{cuL^2}{Q} \qquad (3)$$

where

*c* measured volumetric concentration

*u* reference wind speed at the reference height *L*

*Q* volumetric rate of discharge of the tracer

The following quantities have been extracted from the DRIFT predictions for the two vertical sampling array positions of $x/L$ = 14.9 and $x/L$ = 29.8:

*Kmax*: the maximum centreline concentration over the wind-tunnel measurement height

*K*: the ground-level centreline concentration

*Zc*/*L*: the height of the maximum concentration *Kmax*

The DRIFT predictions have been compared with parametric fits [5] to the wind-tunnel results in [7]. As an example, predictions for a square source with area $7.2L^2$ (denoted Source C) are shown below in Figure 2.

The results [7] indicate that, with some exception noted below, the agreement for Source C generally holds also for the other source sizes and shapes. We infer the following:

- The effect of buoyancy on maximum centreline concentration is well represented.
- The buoyancy at which the transition occurs from ground-based plume to elevated plume is well represented, even for the widest source. An exception is the longest 'Long Source', which shows more rapid lift-off in the wind-tunnel than predicted by DRIFT. This is possibly a result of lift-off occurring over the source which is not well represented by DRIFT's bulk treatment of the plume cross-section.
- The predicted rise of the location of maximum buoyancy is in reasonable agreement with the wind-tunnel data, albeit with a slight tendency to under-predict plume rise. When 'added mass' was included within the DRIFT model equations, insufficient plume rise is predicted.
- For the cases where the plume has lifted-off from the ground, the ground-level concentrations predicted by DRIFT are larger than observed in the experimental measurements. This may, in part, be related to the assumed shape of the elevated plume being axi-symmetric whereas a very buoyant plume may become 'kidney' shaped.
- The plume height *Zc/L* predictions from DRIFT are with zero 'added mass' in the plume vertical momentum equation. Including added mass was found to be detrimental to the agreement with the wind-tunnel data, with added mass suppressing too much the buoyant rise.

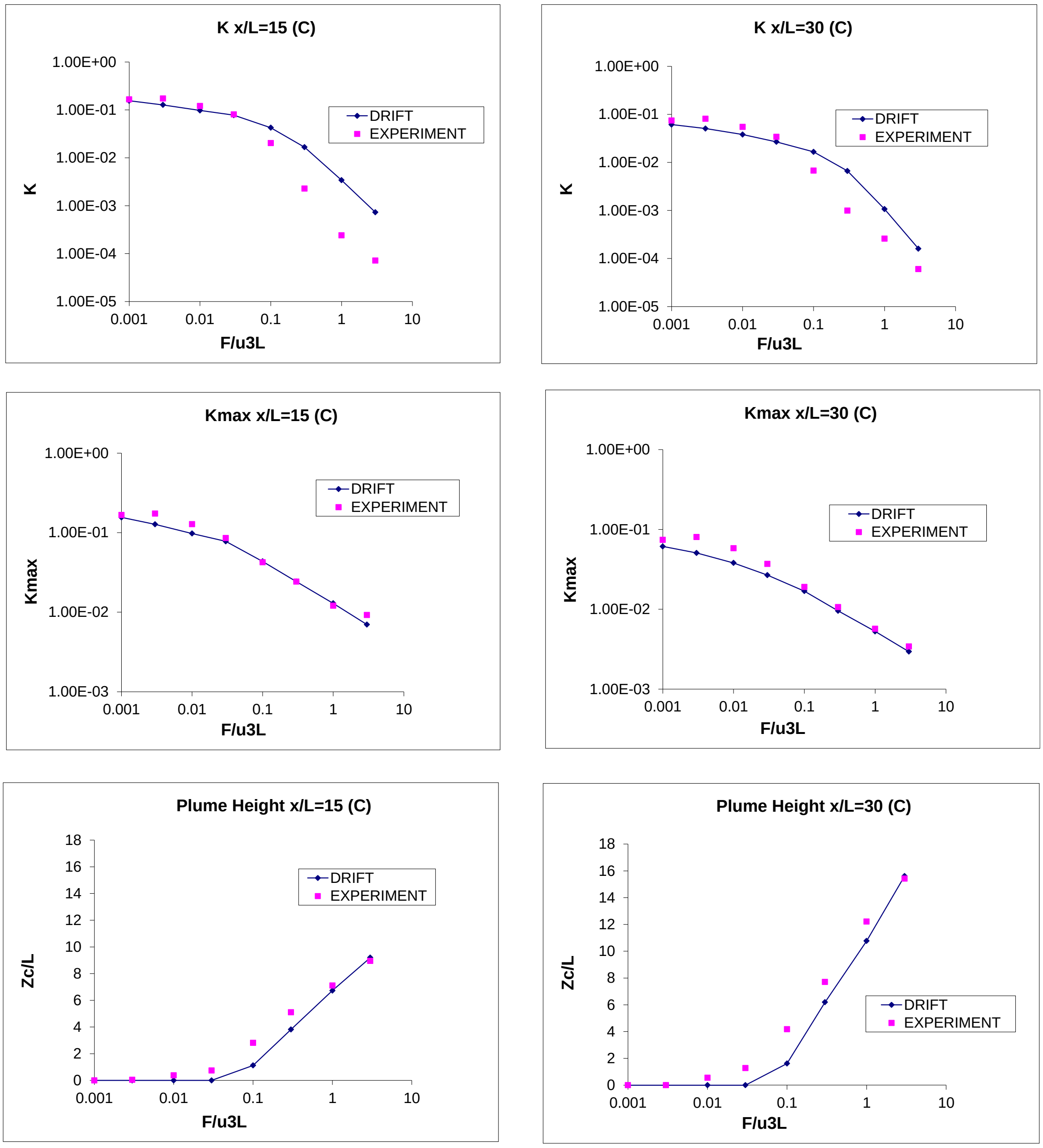


**Figure 2 DRIFT predictions for plume source C**

# Buoyant puffs

## Experimental Conditions

The buoyant puff wind-tunnel experiments [6] investigated lift-off and dispersion behaviour of short duration buoyant releases. The experiments were undertaken in the same wind-tunnel as the plume experiments [5]. Release duration was varied in addition release buoyancy and source shape. Many repeat experiments were required for the buoyant puff releases to due to the inherent variability of puff dispersion.

Three different kinds of sources were implemented for the puff experiments, namely long (G), square (D) and wide (J). The dimensions and identifying letters are given in Table 2. The same length scale ($L$=6.7cm) is adopted for non-dimensionalisation as in the plume experiments.

**Table 2 Source description**

| *Identifying Letter* | *Width y/L* | *Length x/L* | *Area xy/L$^2$* |
|---|---|---|---|
| G | 0.448 | 3.43 | 1.54 |
| D | 3.43 | 3.43 | 11.78 |
| J | 14.33 | 3.43 | 49.19 |

The discharge conditions used for the puff releases are shown in Table 3.

**Table 3 Puff Release Discharge Conditions**

| *Release Identifier* | *$F/u^3L$* | *Release Duration, T (s)* | *Dimensionless Release Duration, uT/L* | *Release Volume $V_p$ (ml)* | *Dimensionless Release Volume, $V/L^3$* | *Wind Speed, u ($ms^{-1}$)* |
|---|---|---|---|---|---|---|
| A | 0 and 3 | 0.8 | 4 | 2000 | 6.7 | 0.32 |
| B | 0 and 3 | 0.2 | 1 | 500 | 1.7 | 0.32 |
| C | 0 and 0.1 | 0.4 | 3 | 130 | 0.4 | 0.5 |
| D | 0 and 0.1 | 0.16 | 1 | 50 | 0.17 | 0.5 |

The same concentration measurement array as for the plumes (see Figure 11) was used.

## DRIFT predictions

The wind-tunnel puff releases have been modelled using DRIFT Version 3.6.15. As for the plume cases, the DRIFT modelling has been undertaken at the wind-tunnel scale.

The puff releases were modelled in DRIFT using two alternative approaches:

- *Finite Duration Release:* The release is modelled as a low momentum area source which is approximated as being steady and continuous over the release duration. DRIFT accounts for the finite duration by including additional longitudinal dispersion (mixing at the front and back edges of the plume segment).
- *Instantaneous Release:* The entire release volume is modelled as being instantaneously released puff. DRIFT's puff model includes longitudinal as well as lateral dispersion.

DRIFT concentration (% vol/vol) predictions have been compared with the wind-tunnel puff results. The following quantities have been compared for the two vertical sampling array positions of $x/L$ = 14.9 and $x/L$ = 29.8:

- *Cmax*: the maximum centreline concentration over the wind-tunnel measurement height range
- *C*: the ground-level centreline concentration
- *Zmax*/*L*: the height of the maximum concentration *Cmax*

The DRIFT predictions are compared with maximum measured concentrations from the wind-tunnel in [7].

As an example comparison Figure 3 illustrate the DRIFT instantaneous model predictions for Source D. The x-axis labels in these figures indicate firstly the release identifier (codes A-D in Table 3) and secondly the buoyancy condition (A, Z and W in Table 1). In these comparisons, the large variability of the wind-tunnel results reported in [6] should be born in mind.

Overall these comparisons indicate:

- The effect of buoyancy on maximum centreline concentration is, in general, well represented and reflects the expected trends – in particular buoyant puffs show more rapid dilution and less buoyant rise than buoyant plumes with the same buoyancy flux.
- Modelling the releases as either finite duration or instantaneous generally produces similar maximum concentration predictions, indicating that the releases are best scaled with total buoyancy, rather than buoyancy flux. However, the DRIFT modelling does show differences in lift-off height between the finite duration and instantaneous models, with the lift-off height from the instantaneous model being in better agreement with the experimental data.
- The model predictions for puff releases are with 'added mass' included as in the model of Turner on which DRIFT's buoyant puff model is based.

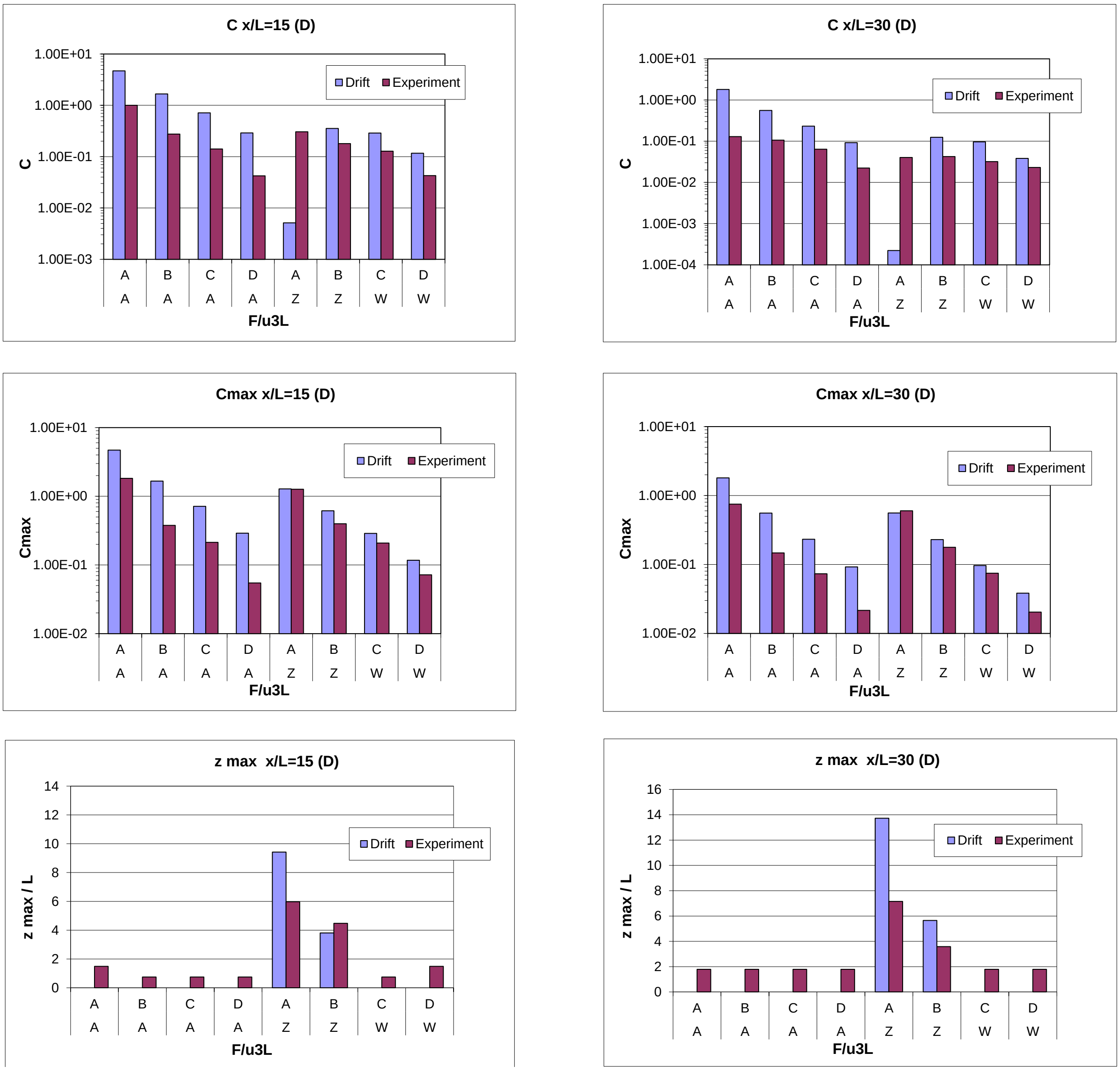


**Figure 3 DRIFT instantaneous model predictions for puff source D**

## HF thermodynamic model comparisons

Schotte [11] measured the temperature change on mixing HF vapour with moist air in a fog chamber for a range of relative humidities. Figure 4 shows the temperature predictions for these experiments using DRIFT Version 3. Also shown in Figure 4 are the experimental data and results from an independently coded spreadsheet model HF-Mixture [9]. The DRIFT Version 3 predictions match almost exactly those from the independent spreadsheet model and are also in excellent accord with the experimental measurements of Schotte.

HF thermodynamic mixing experiments were undertaken under URAHFREP with the aim of extending the range beyond Schotte's [11] and investigating the effects of including iso-butane in the mixture. Details of these URAHFREP thermodynamics experiments are reported in [12]. The mixed streams were initially at a temperature of 294K.

Figure 5 shows DRIFT predictions compared with the URAHFREP HF –moist air mixing data [12]. Again the DRIFT predictions very match those of the HF-Mixture model in [9]. The model predictions also agree reasonably well with the experimental measurements, in particular the minimum and maximum temperatures agree well, despite the experimental measurements showing some deviations and scatter.

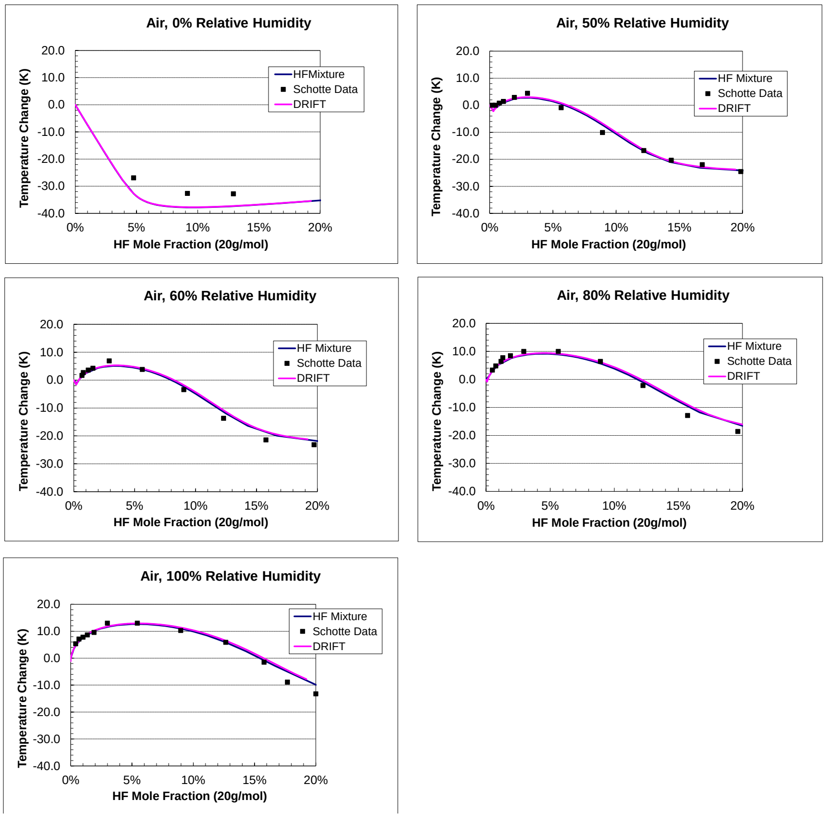


**Figure 4 Temperature change on mixing HF with moist air at 299K – Schotte Data**

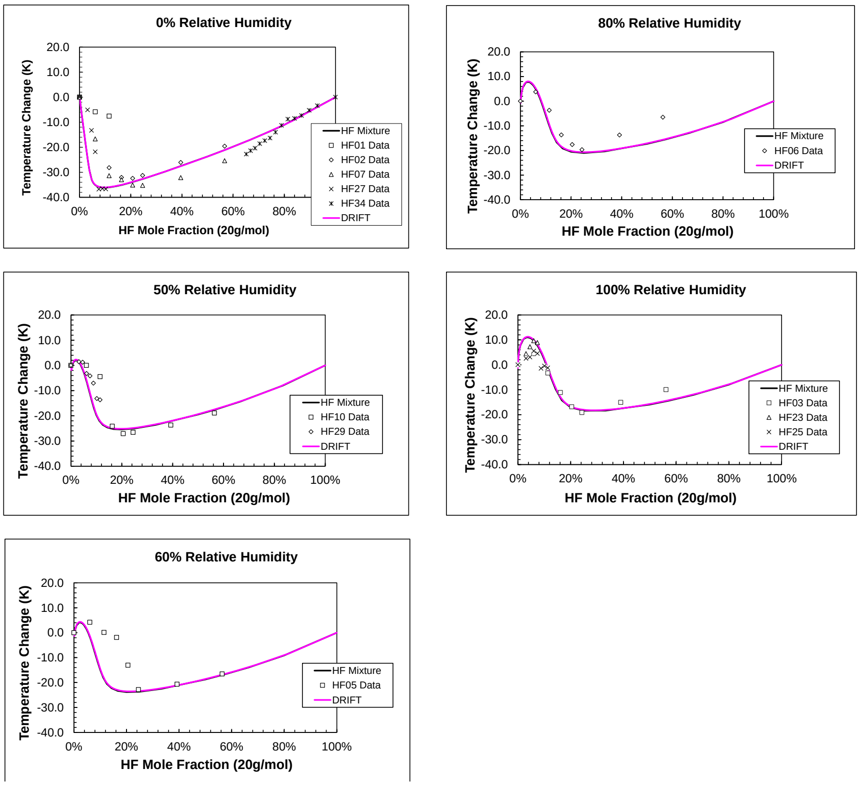


**Figure 5 Temperature change on mixing HF with moist air at 294K – URAHFREP data**

## HF field trial comparisons

The URAHFREP Campaign 2 field trials released anhydrous HF at approximately 0.1 kg/s in different atmospheric conditions. Details of the URAHFREP field trials are reported in refs [3, 13, 14 and 15]. In this section comparisons with predictions from DRIFT Version 3.6.15 are presented.

To match the time averaging of the different concentration measurements, DRIFT results for two averaging times are presented:

- Averaging of the duration of the discharge (appropriate for CEA filters)
- Averaging over 1 s (appropriate for other measurements)

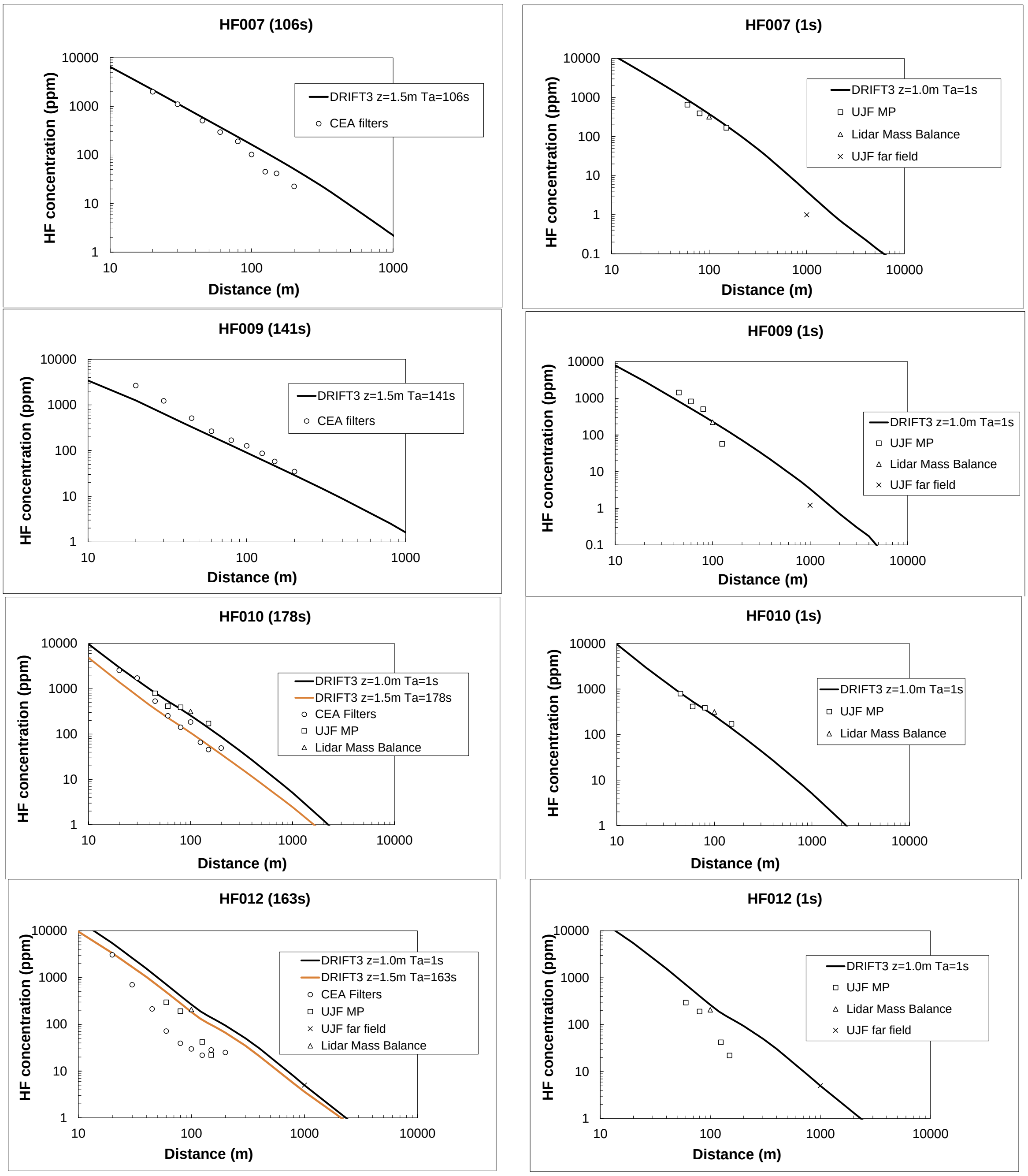


**Figure 6 Comparison of DRIFT predictions with URAHFREP Campaign 2 concentration measurements**

Figure 6 compares concentration predictions from DRIFT 3.6.15 with field measurements for the field trails HF007, HF009, HF010 and HF012. Of the URAHFREP field trials, only HF012 was under conditions where enhanced buoyancy may affect dispersion. However, even for HF012 these HF buoyancy effects may be masked by convective atmospheric conditions.

The experimental data for HF012 shows a significant dip in concentration between 10m and 200m from the release point compared with the DRIFT predictions. DRIFT also shows a dip at this distance, but this is much smaller than dip in the data. DRIFT is predicting HF induced buoyant rise here, but the effect of this is much less marked than in the experimental data. There is evidence from smoke observations in [13] that the observed plume rise in HF012 is, at least in part, due to an atmospheric updraft in low wind unstable conditions. The effect of a single atmospheric updraft is not modelled in DRIFT 3 which rather includes the effect of sampling *both* updrafts and downdrafts based on a probability density model. The plume rise effect for HF012 is transient with DRIFT showing good agreement with the far field measurement at 1000 m.

## Lift-off sensitivity to relative humidity

Due to site safety considerations, the URAHFREP field trials released only approximately 0.1 kg/s of anhydrous HF. Greater buoyancy effects on dispersion are expected for larger release rates. Ref [16] considered the potential effect on buoyant lift-off of varying release rate and atmospheric conditions over a wider range. As an illustration, Figure shows DRIFT Version 3.6.15 side elevation predictions for a 1 kg/s flashing release of anhydrous HF from a 4 mm diameter hole in F2 (Pasquill stability F; 2m/s wind speed at 10m height) weather conditions with an ambient temperature of 293 K for relative humidity values of 40%, 50%, 60%, 70%, 80%, 90% and 100%. The roughness length for these runs is 0.1m. The displayed contour corresponds to a toxic dose of 12,000 ppm.min which is equal to HSE's Dangerous Toxic Load for Specified Level of Toxicity (SLOT DTL) for HF.

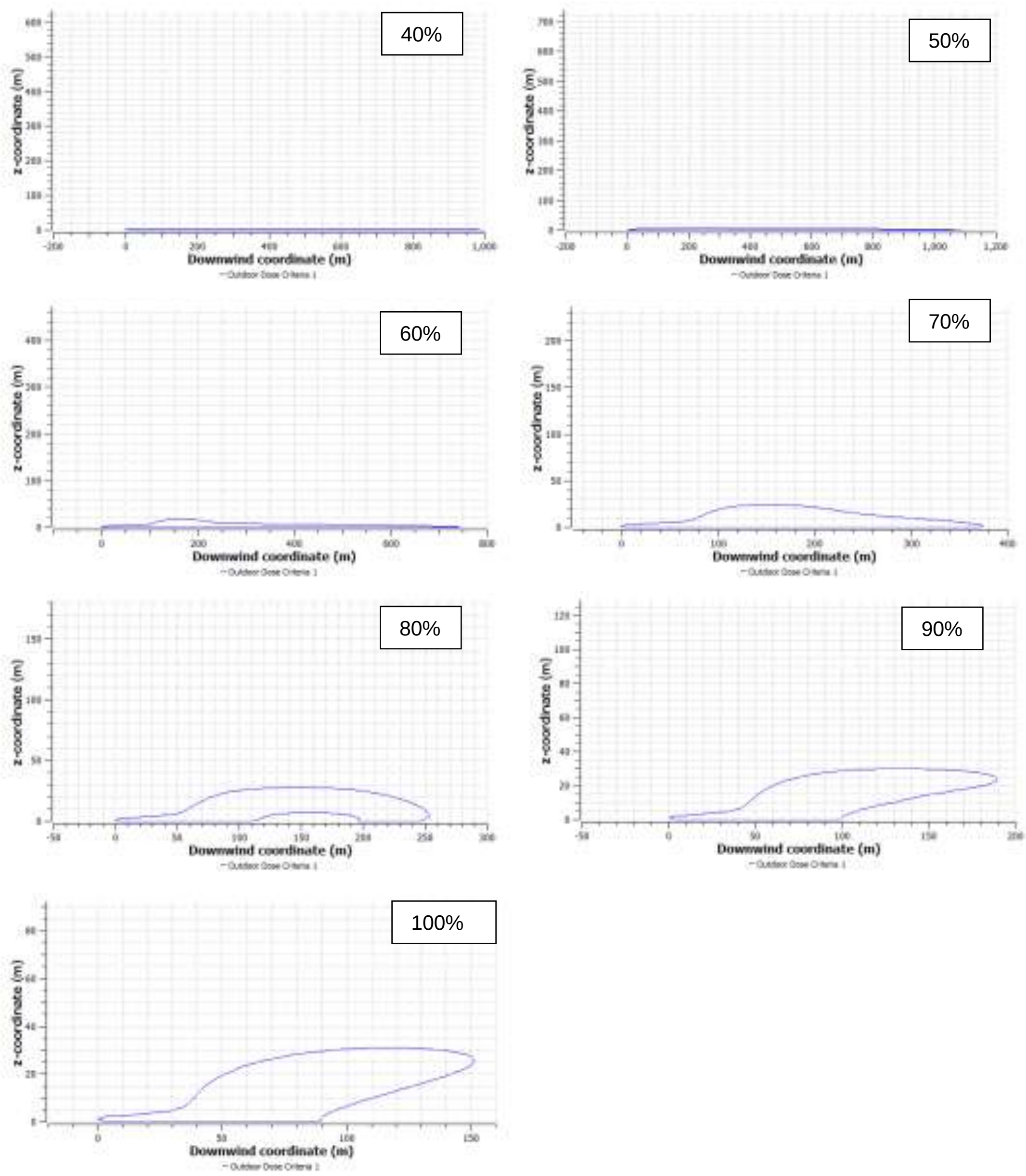


**Figure7: Relative humidity dependence for 1 kg/s release of HF in F2 weather. Side elevation contours of SLOT DTL.**

For the specific release example shown here, the downwind range to SLOT DTL varies from approximately 1100 m to 150 m depending on atmospheric humidity. This illustrates the potential for considerable shortening of hazard range due to HF-water interaction induced buoyant lift-off in low wind, humid conditions. Ref [16] showed that the buoyancy effect becomes more marked for larger release sizes and how this may be negated by the presence iso-butane aerosol.

## Concluding remarks

This study indicates that the buoyant enhancements incorporated into DRIFT Version 3 perform reasonably well compared with experimental data. The influence of buoyancy on maximum concentration appears to be well represented. The prediction of other parameters, e.g. buoyant plume and puff rise is more variable, but appears reasonable overall. Ground-level concentration predictions for lifted-off plumes are generally higher than the wind-tunnel measurements.

Comparison with experimental data indicates that the thermodynamic behaviour of mixtures of hydrogen fluoride with moist air is well established. Extending models to include other components, e.g. iso-butane is less certain, although URAHFREP measurements support iso-butane acting as a diluent which may counteract buoyancy generation.

The comparisons with URAHFREP field trials data show that DRIFT Version 3 can adequately represent these real HF releases. Using DRIFT Version 3, much larger HF releases than in the URAHFREP field trials can now be modelled in humid, low-wind conditions – the results from which depend on DRIFT's buoyant lift-off model, which is shown here to be in reasonably good agreement with wind-tunnel data. The sensitivity of model predictions to atmospheric humidity should be considered when selecting representative scenarios for risk assessment involving releases of anhydrous HF.

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