Report

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Model Predictions Compared with URAHFREP Campaign 2 Field Trial Data

A Deliverable produced under Work Package 7 of the EC URAHFREP Project, Contract No. ENV4-CT97-0630

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Executive Summary

The occurrence and quantification of the mitigation of anhydrous hydrogen fluoride (AHF) clouds due to buoyancy generation is currently very uncertain. The EC URAHFREP research programme is aimed at reducing the uncertainties to enable more reliable estimates to be made of the hazards associated with accidental hydrogen fluoride releases.

Field trials have been conducted under URAHFREP involving the medium scale (~0.1kg/s) release and dispersion of AHF under normal European (humid) atmospheric conditions. This report details comparison of data from these field trials with predictions of HF dispersion models. The dispersion models are the AEAT/HSE models EJECT and DRIFT. These models employ HF thermodynamic models which have been shown to adequately represent chamber mixing studies. The dispersion models have also recently been enhanced in the light of URAHFREP wind-tunnel studies. The findings of these wind-tunnel experiments are used in this study as a guide to assessing the possible lift-off implied by the model predictions.

Initial comparisons show many of the URAHFREP field trials to be dominated by passive dispersion. A review of the passive dispersion model in DRIFT for continuous sources has led to a modification of the lateral passive spreading model. A simple model to account for the effect of averaging time on concentration has also been introduced. A selective re-validation of the model has been conducted, before going on to compare the new model predictions with the URAHFREP field trials.

The URAHFREP field trials indicate that out of the 12 trials conducted plume lift-off possibly occurred for only one trial (HF012). Dispersion model predictions and lift-off criteria based on wind-tunnel data are in accord with these findings. Only a selection of the trials have been modelled, but findings are expected to apply more widely due to the similarity of many of the release and ambient conditions. The influence of ambient conditions on concentration are predicted to be dominant over HF thermodynamics, except possibly for trial HF012. The models indicate that (due to low windspeed and high humidity) the generated buoyancy may be sufficient to lead to lift off for Trial HF012. Some caution is necessary since the lift-off criteria employed do not include the effect of ambient convection which may be the dominant mechanism for the lift-off which was observed for HF012. Downdrafts in ambient convection may also lead to clouds, which otherwise would be expected to lift-off, remaining ground based.

Theoretical modelling studies have also been undertaken. These are aimed at showing the effects of releasing larger quantities of HF and of releases under different atmospheric conditions. Not surprisingly increasing the size of the release increases the importance of gravitational effects, including the potential for buoyant lift-off. Similarly more stable atmospheric conditions are predicted to encourage lift-off.

Contents

1   Introduction

Anhydrous hydrogen fluoride (AHF) is commonly stored and used in the bulk in chemical and nuclear industries [1]. Notably large amounts of AHF are used as a catalyst for the alkylation process in the petroleum industry. The high toxicity of hydrogen fluoride [2] means that accidental releases have the potential to lead to significant hazards to both people and the environment. Reliable estimation of the dispersion behaviour of anhydrous hydrogen fluoride is therefore of considerable importance, but this behaviour is complicated by the thermodynamics of mixing AHF with moist air. HF thermodynamic models (e.g. refs. [3] and [4]) indicate that for ambient humidities frequently encountered in European climes, HF clouds which are initially heavier-than-air may become lighter-than-air as the cloud disperses (ref. [4]). The influence of such buoyancy generation may be to mitigate the hazard as compared with a non-buoyant release, due to enhanced dilution and possibly also buoyant lift-off of the cloud from the ground.

The occurrence and, in particular, the quantification of the mitigation of HF clouds due to buoyancy generation is currently very uncertain. Firstly, the generation of buoyancy is based on the predictions of theoretical thermodynamic models that make certain simplifying assumptions which need to be validated [4]. Secondly, the understanding of the dispersion behaviour of ground based buoyant releases is somewhat limited, even for buoyancy conserving plumes, let alone for plumes with changing buoyancy [5]. Thirdly, there is the lack of field data for releases of AHF under humid conditions with which to validate models. The EC URAHFREP research programme, of which the work here is a part, is aimed at reducing these uncertainties to enable more reliable estimates to be made of the hazards associated with accidental AHF releases.

Earlier work [6] under URAHFREP confirms the validity of existing HF thermodynamic mixture models, at least for well mixed equilibrium conditions. Recent wind-tunnel studies [7,8] have led to an improved understanding of lift-off behaviour and give guidance on the selection of suitable lift-off criteria for buoyant clouds. These lift-off criteria shall be used in this study as a guide to assessing the possible lift-off implied by the model predictions.

In this report we are concerned with the validation of HF dispersion models against URAHFREP Field Trial data. The dispersion models are the AEAT/HSE models EJECT [9] and DRIFT [10]. The models have also recently been revised in the light of URAHFREP wind-tunnel and thermodynamic studies [6,11]. In particular we are interested in whether the current models in conjunction with the aforementioned lift-off criteria are in accord with the observed lift-off and dilution behaviour in the Field Trials.

2   URAHFREP Field Trials

During a two week period in August 2000 a total of 12 trials were conducted at the DERA Porton Down site [12].   Extensive data are available from these trials. It is intended that these data will be transferred into the REDIPHEM database [13]. In the mean time we have to rely on data and draft reports made available by partners. No major changes are however envisaged for the final versions.

We report in Section 2 on our analysis of the experimental data for the purposes of performing comparisons with model predictions. As is often the case with a major set of field trials, unforeseen delays mean there is limited time for modellers to assimilate and do real justice to the quality data eventually produced. We have coped with this situation by considering only a subset of the trials for comparison and by undertaking a fairly crude analysis of the data. Since, as we shall see below, many of the earlier trials were under similar conditions, we have been able to select a few trials which cover most of the significantly different release and ambient conditions.

2.1   RELEASE CONDITIONS

Each trial consisted of a horizontal pressurised release of AHF liquid. The release height was 1.2m and directed in the nominal downwind direction. The release rig was designed to give a constant release rate of HF during each trial. A summary of the HF release conditions as reported by HSL [14] are reproduced in Table 1 below. The quoted release duration in Table 1 is the duration over which the release rate was held steady[1].   The pressure is measured by a sensor close to the exit. No pressure or temperature information is available for trial HF003 due to a data logging problem. For two trials, HF009 and HF011, an isobutane jet was mixed with the HF jet. The isobutane release conditions for these trials are summarised in Table 2. For further details of the release rig, its operation and related measurements the reader is referred to the HSL report [14].

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[1] For a short period before and after there was a small amount of HF released. We shall ignore these quantities in our modelling studies.

Trial	HF Release				
	diam.	Rate	Press (exit)	Temp (exit)	Duration
	mm	kg/s	bar g	°C	s
HF001	1	0.061	4.13	18.60	85
HF002	1	0.074	6.67	18.09	131
HF003	1	0.15			102
HF004	4	0.084	8.70	16.59	184
HF005	2	0.085	8.83	15.84	180
HF006	2	0.083	8.66	19.11	187
HF007	2	0.145	3.78	18.78	106
HF008	3	0.104	4.04	13.86	145
HF009	2.5	0.108	4.70	17.90	142
HF010	2.5	0.113	4.91	10.84	179
HF011	2.5	0.111	4.78	13.03	188
HF012	2.5	0.123	5.74	7.98	163

Table 1. Summary of HF Release Conditions for the URAHFREP Field Trials.

Trial	Isobutane Release			
	diam	Rate	Press (exit)	Temp (exit)
	mm	kg/s	bar g	°C
HF009	3	0.103	4.75	12.85
HF011	3	0.99	4.84	10.75

Table 2. Isobutane Release Conditions for the URAHFREP Field Trials.

2.2   METEOROLOGICAL CONDITIONS

2.2.1   Roughness Length

Figure 1 is reproduced from the Risoe report [12] showing that the roughness length is observed to vary with the 10m elevation windspeed.   The reason for the roughness length increasing with decreasing windspeed is not understood. Based on the assumption that z_0 enters only as log z_0, Risoe recommend a value of 2cm. For AEAT model comparisons we adopt a z_0 of either 2cm or 10cm, depending on which gives the closest match to the observed 10m windspeed when the observed friction velocity, u_* and Monin-Obukhov length, L are input to DRIFT.

As an example consider trial HF007. Using u_*=0.39m/s and L=-34m, DRIFT's atmospheric profiles [10] indicate the following 10m windspeeds

u_{10} = 6.1m/s using z_0=2cm
u_{10} = 4.5m/s using z_0=10cm

The observed 10m windspeed for this trial is 4.2m/s which is closest to the DRIFT value with z_0=10cm, therefore we would adopt z_0=10cm for this trial. Selecting the z_0 values in this way gives values which are generally in accord with the trend in Figure 1.

2.2.2   Release Conditions

Meteorological conditions during the trials were measured by Risoe and are summarised in their report [12]. Information required for running the AEAT models has been extracted from the Risoe report and are summarised in Table 3. At the time of writing, the Risoe draft report does not give meteorological conditions for HF001 and HF002. These are therefore left blank in Table 3.

Table 3 indicates that all the releases were conducted during either effectively neutral or unstable conditions.

Trial	U (2m)	u*	rh (2m)	T (2m)	L
	m/s	m/s	%	°C	m
HF001					
HF002					
HF003	3.8	0.38	80	18.3	-141
HF004	5.2	0.24	89	20.0	-27
HF005	4.8	0.50	80	19.8	-434
HF006	5.1	0.41	74	21.2	-75
HF007	3.4	0.39	53	19.9	-34
HF008	2.8	0.21	76	17.4	-6.3
HF009	6.5	0.50	46	21.6	-69
HF010	4.0	0.42	83	14.5	-220
HF011	4.6	0.49	69	16.7	-155
HF012	1.3	0.14	92	11.8	-18

Table 3. Meteorological Conditions for each URAHFREP Field Trial. U, rh and T are the windspeed, relative humidity and temperature measured at a height of 2m. L is the Monin-Obukhov length.

2.3   FIELD TEMPERATURE MEASUREMENTS

Time series temperature measurements are available from thermocouple arrays in the near field (5m-25m from the release point). The locations of the thermocouples are shown in Figure 2.

The response time of the thermocouples is quoted as being approximately 1.5s and data were collected at a frequency of 1Hz. Measurement problems due to thermocouple damage from HF and cold junction errors mean that only temperature differences from the ambient values are viewed as being reliable [14].

HSL has performed some analysis of the temperature data. Their analysis involved dividing the thermocouples into groups based on the measurement height and distance from source. The highest reading in each group was then selected and averaged over the duration of the release. This method removes some of the effects of plume meander. The results of the HSL analysis are given in Table 4 below. There are no data available from HF003.

Distance (m)	5				20	25		
Height (m)	0.25	0.5	1	1.5	1	0.5	1	1.5
HF001	0.11	0.54	1.12	0.99	0.16	0.34	0.35	0.38
HF002	-1.06	0.54	1.31	1.65	0.32	0.6	0.52	0.43
HF004	5.57	5.71	6.13	6.35	2.14	2.58	2.38	1.31
HF005	4.62	4.97	5.14	5.62	1.4	1.92	1.7	1.11
HF006	4.54	4.14	4.88	4.86	1.01	0.81	0.9	0.59
HF007	-21.08	-8.13	-2.43	0.33	1.27	1.65	1.73	1.52
HF008	-27.95	-5.54	2.44	3.96	2.28	3.12	2.97	2.62
HF009	-26.67	-18.65	-8.48	-4.84	0.39	0.35	0.53	0.22
HF010	-17.62	-1.54	3.54	4.57	1.73	2.76	2.49	1.77
HF011	-2.48	0.57	2.42	2.85	1.57	1.65	1.41	0.98
HF012	-6.15	2.18	3.94	3.61	3.78	2.87	3.02	2.23

Table 4. Peak temperature changes (K) measured by field thermocouples averaged over each release.

2.4   FIELD CONCENTRATION MEASUREMENTS

2.4.1   CEA Chemical Filters

CEA have provided estimates of concentration based on HF loading of chemical filters placed in the near field. The filters were placed at heights of 1.5m or 3m above ground and located in arcs at distances of 20m, 30m, 45m, 60m, 80m, 100m, 125m and 200m. Figure 3 illustrates the arcs and defines the polar co-ordinate frame used for locating the sensors. The sensors are located centred around the 30° line, since this is the angle for the ideal wind direction of the experiment.

CEA quote [16] the HF concentration based on the amount of air sampled by the filter during its operation. The filter pumps were started when the steady release started and ended when steady release started to decay. This procedure will underestimate the actual concentration averaged over the full duration of the release due to the time delay in the cloud reaching the measurement location. Underestimation will be largest for the largest travel times, ie for the trials with the lowest wind speeds and farthest located sensors. For our comparisons with model predictions, we have attempted to correct for this by assuming the effective advection speed of the cloud is approximately equal to the 2m windspeed. This is supported by the LIDAR observations at 100m (see below).

Ideally we would like to compare model predictions for centreline concentration (and cloud width) with measured data. With this in mind, we shall compare model centreline predictions with the maximum value observed on each arc. There are insufficient measurements in some arcs to be confident that the maximum measured value relates (even approximately) to the centreline.

2.4.2   UJF Spectroscopic Devices

Laboratoire de Spectromètrie Physique, University de Joseph Fourier made concentration measurements with high quality spectroscopic detectors [16].

In the near field 15 short path devices, called multipoint detectors (MP), were employed. The location of the detectors is given by the ● symbols in Figure 3. The devices have a fast response (~1s averaging time) and are in principle capable of measuring HF concentrations between 2 ppm and 2% by vol. Data were recorded at a frequency of 1Hz. Unfortunately, due to a software bug, concentrations higher than 2200 ppm were discarded by the recorder and replaced with the missing value data marker.

At 1km downstream concentrations were obtained from two cavity ring down spectrometers (CRDS) separated by 10m. These have a detection range between 20 ppb and 30 ppm and similar averaging time to the multipoint detectors, and also measured water vapour concentrations.

The problem in using the UJF concentration measurements for comparison with model predictions is in knowing whether they can be taken to be representative of the plume centreline. Meander of the plume means that it is unlikely that a given sensor will remain at the 'instantaneous plume' centre, or even within the plume. For our comparisons we extract the maximum (peak) concentration measured at a particular location. We compare the maximum of these values on each arc with the model predictions. We recognise that such an approach is dependent on the detector response time and is prone to selective statistical fluctuations which are higher than the true average maximum value. It does however serve to show how the model centreline concentration estimates relate to the maximum observed concentration at each distance.

2.4.3   LIDAR Measurements

Risoe scanned the plume cross-section at 100m downstream using a rapid scanning LIDAR [12]. The LIDAR measures scattering from the seeded cloud[2]. Absolute concentration is not measured by the LIDAR. Risoe present results for various moments of the measured concentration distributions, including cloud centroid height, vertical and lateral standard deviations. Risoe also give results from a "moving frame" analysis of the data which effectively subtracts the contribution of the time varying lateral motion (meander) of the cloud centroid.

The LIDAR also scanned passive smoke plumes released immediately following the HF releases. The LIDAR provides a good means of assessing whether the plume has lifted off and on the differences between the HF and passive releases in very similar meteorological conditions.

We shall attempt to estimate absolute concentration from the LIDAR results in [12] by performing an approximate mass balance calculation. We give the basis of these calculations below.

The LIDAR measurements show that after subtracting plume meander (using a moving frame analysis) the lateral distribution is approximately Gaussian:

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[2] The cloud was seeded by introducing a small amount of ammonia producing NH_4F aerosol.

$$F_h = \exp\left[-\left(\frac{y}{b}\right)^2 \right]$$ (1)

b is a lateral length scale (which is related to σ_y) an y is the lateral distance from the centreline.

For releases which remain grounded (all except HF012), we shall assume that the vertical concentration distribution may be approximated by

$$F_v = \exp\left[-\left(\frac{z}{a}\right)^s \right]$$ (2)

z is the vertical co-ordinate, a is a vertical length scale, which is related to σ_z and the centroid height $\overline{Z}$ defined by

$$\overline{Z} = \frac{\int_0^\infty z F_v dz}{\int_0^\infty F_v dz}$$ (3)

and

$$\sigma_z^2 = \frac{\int_0^\infty (z - \overline{Z})^2 F_v dz}{\int_0^\infty F_v dz}$$ (4)

s is a vertical profile parameter describing the shape of the vertical distribution.

DRIFT's profiles [10] in the passive limit are of the above form. The profile parameter s in DRIFT is 1 for neutral conditions, but in general depends on atmospheric stability ($\overline{Z}/L$). For small $\overline{Z}/L$, the regime for the observations here, s is close to the neutral value. We therefore assume a value of unity, but note that based on published data values possibly up to s=1.5 might just as well be used [17].

To perform a mass balance we also need an estimate of the 'effective plume velocity', $\overline{U}$. Strictly we should obtain this by an integration of the velocity profile weighted by F_v. For non-neutral profiles this would require numerical integration or fitting to power law profiles. We shall avoid such complications here by utilising the observation [12] that the plume arrival time at the LIDAR is well approximated by the observed 2m windspeed, u(2): ie

$$\overline{U} = u(2)$$ (5)

Integrating over the above profiles gives the relation:

$$m_{HF} = c_m 2\sqrt{2}\sigma_y \overline{Z}\,\overline{U} \qquad (6)$$

where m_{HF} is the HF release rate (kg/s) and c_m is the maximum HF concentration (kg/m^3).

When the plume is elevated we assume Gaussian shapes for both lateral and vertical distributions.

$$m_{HF} = c_m 2\sqrt{\pi}\sigma_y \sigma_z \overline{U} \qquad (7)$$

Now for $\overline{U}$ we use the windspeed at the centroid height $\overline{Z}$. In the above we have neglected any contribution arising from so-called reflection at the ground. We justify this on the grounds that for the one trial (HF012) to which we apply this form, $\overline{Z}$ =19.29m, whereas σ_z =7.46, ie the contribution to maximum centreline concentration from reflection terms would be negligible.

Equations (6) and (7) are used to estimate the maximum concentration c_m from the moving frame average values given in the Risoe report [12].

3   Model Predictions

In Section 2 we discussed the URAHFREP Field Trial data selected and analysed for comparisons with model predictions. Risoe's analysis of LIDAR data shows that for all trials, except HF012, the plumes are fully grounded at 100m, and that there is no evidence of enhanced mixing due to HF thermodynamics – the plume profiles are essentially indistinguishable from the passive plumes. The HF012 release is for the lowest windspeed of all the trials and in conditions of rapidly changing meteorology – the conditions becoming increasingly unstable. The LIDAR scans show the plume concentration maximum at a height of about 20m at 100m distance. However, the corresponding passive smoke plume also shows a similar degree of lift-off. Risoe's analyis shows the HF plume is slightly higher than the smoke plume, but it is difficult to show that this difference between HF and smoke is significant. One of the main aims of our modelling study is to see if these observations are consistent with model predictions.

In Section 3 we show, for selected trials, comparison of these data with model predictions. The dispersion models are the AEAT/HSE models EJECT [9] and DRIFT [10]. EJECT is a two-phase jet model which provides the source term for the DRIFT dense gas dispersion model. During the course of our comparisons we have looked in more detail at DRIFT's passive model and made some minor modifications. The details are given in Appendix 1. In this Chapter we shall therefore first report the initial comparisons (Section 3.1) with the model without these changes, summarise the changes to the model (Section 3.2) and repeat and extend the comparisons with the predictions of the revised model (Section 3.3).

3.1   INITIAL COMPARISONS

We report here initial comparisons of model predictions with experimental data. The model results are from EJECT Version 2.10 and DRIFT Version 2.26 [10,9,18]. These versions differ from earlier versions in two main respects:

(i)   Bugs in the DRIFT HF (and ammonia) thermodynamic model have been corrected. These bugs resulted in earlier versions of EJECT and DRIFT giving slightly lower temperature rises in high humidities than in the corrected versions. The model predictions are now well in accord with HFMIXTURE, an earlier coding of the HF thermodynamic model called WETAHF, and most importantly the HF thermodynamic measurements [6].

(ii)   Incorporation of enhanced dilution when the ground based cloud is buoyant. Earlier versions assumed passive dilution when the cloud became less dense than the ambient air. An entrainment function derived from the wind tunnel data of Hall et al [7,11] is now used when the cloud is buoyant.

3.1.1   Modelling the jet phase of the release

The jet phase of the release is modelled using the two-phase jet model EJECT.

EJECT takes as input the mass flow rate, liquid fraction, temperature and pressure at the exit. The mass flow rates and exit pressures as summarised in Table 1 are input directly to EJECT. In all the field trials HF liquid was released at temperatures below its normal boiling point, hence it did not flash, rather formed a liquid spray. EJECT cannot model such spray releases. This has been overcome by adjusting the exit temperature to just above the HF normal boiling temperature – which introduces a very small amount of flashing and resets the source temperature after flashing to be the normal boiling point. The HFMIXTURE [6] thermodynamic model does not have such restrictions. Figure 4 shows the effect on mixture temperature of altering the source in this way. The conditions for Figure 4 are based on those for trial HF012. This comparison indicates that a difference of over 10K in temperature at the source leads to a difference of just about 2K in the temperature minimum. The temperature maximum is almost unchanged. This is not too surprising since the most significant contributions to the heat balance are the latent heats of vaporisation, oligomerisation and heat of mixing. We shall therefore use EJECT with these elevated temperatures.

For atmospheric conditions EJECT takes as input the Pasquill stability category, together with the roughness length and windspeed at a reference height. These are then converted (by the model) to friction velocity and (inverse) Monin-Obukhov length using the method in [19] based on Golder's charts [20]. The Pasquill categories for the URAHFREP trials have been determined by the inverse of this procedure.

3.1.2   Modelling the ground based plume

Unlike EJECT, DRIFT allows direct input of friction velocity and (inverse) Monin-Obukhov length. These have been set according to Table 3. For our comparisons we shall neglect the modelling of deposition of HF from the plume. This most closely reflects the use of the model in risk analysis and may not be too important in the near field (except possibly for HF003 which was observed to deposit liquid on the ground). Deposition may however be significant over long distances.

3.1.3   Inferring plume lift-off behaviour

URAHFREP wind-tunnel studies [7] indicate that lift-off of ground based constant buoyancy plumes is described by a lift-off parameter related to $F/u_{ref}^{3}W$ where

$$F = \frac{1}{\pi} g \frac{(\rho_a - \rho_s)}{\rho_a} \dot{V}_s \qquad (8)$$

is the buoyancy flux, g is the acceleration due to gravity, ρ_a is the ambient density, ρ_s the buoyant gas density, $\dot{V}_s$ the buoyant gas volume flux, W is the width of the plume and u_{ref} is

the wind speed at a reference height. A possible alternative lift-off parameter [5] is the plume bulk Richardson number Ri_* defined by

$$Ri_* = g \frac{(\rho_m - \rho_a)H}{\rho_a u_*^2} \tag{9}$$

where H is the effective depth of the plume, ρ_m the density corresponding to the concentration maximum and u_* is the atmospheric friction velocity.

Mathematical modelling studies [11] indicate that simple 'free' plume (integral) models have difficulties in representing the suppression of plume rise for wide sources. To avoid these modelling difficulties, we shall assess the likelihood of lift-off of the URAHFREP Field Trial releases using the lift-off parameter values predicted by the dispersion models and compare with wind-tunnel observations of buoyant plumes at these parameter values.

Based on the correlation given by Hall and Walker [7], and an estimation of Ri_*, ref.[11] gives the following information:

- The first onset of plume rise, defined by the point where the concentration maximum leaves the ground, occurs for $F/u^3W \sim 0.01$, which is equivalent to the point where $Ri_* \sim -2$.

- The ground level concentration falls to 10-20% of the maximum when $F/u^3W \sim 0.035$, equivalent to $Ri_* \sim -10$

- For $F/u^3W > 0.3$, equivalent to $Ri_* < -70$, the ground level concentration is generally less than 5% of the maximum.

We shall attempt to interpret our model predictions using these values.

The validity of this approach for HF releases in non-neutral atmospheric stability conditions is not without question, as we shall discuss briefly below.

Wind-tunnel lift-off studies involve only buoyancy conserving clouds under neutrally stable atmospheric conditions. It is not immediately obvious that these wind-tunnel results are applicable under different release and ambient conditions. The hope of more general applicability arises if the dependence on lift-off parameter results from 'local' influences (e.g. the local balance of forces on the integral plume), rather than non-local influences (such as the trajectory behaviour of the plume) which may differ for non-buoyancy and buoyancy conserving plumes. This distinction is less important if buoyancy changes slowly compared with the lift-off time-scale. For non-buoyancy conserving plumes, wind-tunnel studies might be more applicable to determining *whether* plume lift-off occurs, rather than in determining how high the buoyant plume will rise. Plume rise after lift-off may be more strongly influenced by the changing buoyancy in an HF plume and better modelled using a plume model.

There is also the possibility that the vertical and lateral distributions of buoyancy within an HF plume differ from a buoyancy conserving plume, and that this may lead to different lift-off behaviour. Within the context of integral modelling, even if the distribution of buoyancy within the cloud could be determined, which in itself would be far from straightforward, it would not then be known how that affected dispersion. It is worth noting that other non-buoyancy conserving clouds e.g. dense vaporising aerosol clouds are successfully described by simple integral models. We therefore do not pursue this problem further.

Another factor potentially influencing lift-off is atmospheric stability. Wind-tunnel observations are based only on neutrally stable atmospheric conditions. Unstable conditions enhance vertical mixing, whilst stable conditions suppress vertical mixing. An approach based on the wind-tunnel behaviour alone may overstate lift-off in unstable conditions, where downdrafts in ambient convection may lead to clouds remaining ground based, which otherwise would be expected to lift-off. Conversely, it is possible that plumes which, due to vertical mixing, do not lift-off in neutral atmospheric stability may lift-off under stable conditions. We are currently unable to quantify the influence of atmospheric stability on lift-off, but note these possible effects.

Let us now consider comparisons with URAHFREP Field Trials data.

3.1.4   Trial HF007

Trial HF007 is a 0.145kg/s release of HF under unstable, low humidity conditions, with a 10m windspeed of 4.2m/s.

DRIFT predictions for ground-level centreline concentration for Trial HF007 are shown in Figure 5. The experimental data points, derived following the procedures discussed in Section 2, are also shown in the Figure.

There is a clear difference between the CEA filter concentrations and those determined from short time averaged UJF and LIDAR mass balance data. That this difference remains after attempting to correct for arrival and departure time effects, indicates that the difference is most likely due to the longer time average for the chemical filters which includes the effect of plume meander which has been 'removed' from the other measurements. This supposition is further supported by comparisons undertaken by CEA and UJF. These comparisons show the UJF MP generally give similar concentrations to coincident CEA filters when averaged over the same (chemical filter sampling) period.

DRIFT's ground level centreline predictions appear to be in closest accord with the higher concentration data, rather than the CEA filter data.

Figure 6 shows the effect of specifying different receptor heights in DRIFT. For comparison the UJF sensors are at a height of 1m, and the CEA filters are at 1.5m at distances up to and including 100m and 3m for subsequent distances. The effect of receptor height is probably too marked in DRIFT in the near field due to the abrupt transition the model makes from the airborne jet to the grounded plume.

For this trial the predicted Ri_* values remain positive, indicating that the relative humidity is too low for the cloud to become less dense than air. Downstream of the momentum jet region, the maximum predicted value is $Ri_* = 0.9$ occurring at around 40m. At 100m $Ri_* = 0.3$. Such low values for Ri_* indicate predominantly passive behaviour. This is confirmed by running DRIFT using a passive source with the same molar flux. As shown in Figure 7, this passive DRIFT run gives almost identical concentrations to the run utilising HF thermodynamics.

We conclude that, apart from the initially dense jet phase, the HF007 release may be treated as being passive cloud. Perhaps this should not be too surprising, given the size of the HF release, and the fact that the release is under unstable atmospheric conditions.

3.2   REVIEW AND MODIFICATION OF DRIFT'S PASSIVE PLUME MODEL

Our comparison of DRIFT predictions with concentration measurements for Trial HF007 indicate that DRIFT is in closest agreement with the peak or short time averaged data (UJF and LIDAR mass balance). A cursory comparison with the other URAHFREP trials indicates that this is generally the case. Is this what we should expect from DRIFT's passive model?

The time averaging in DRIFT is wholly implicit, and is based on the entrainment parameter values adopted by the model. Refs. [10,18] indicate that, in the passive limit, the appropriate time averaging is roughly the 15min sampling time discussed by Businger et al [21]. Based on this, one might (naively) expect that DRIFT's predictions should be lower than the peak or short time averaged values. This does not appear to be the case.

In an attempt to resolve these issues DRIFT's passive plume model is briefly reviewed in Appendix 1. From the review (see Appendix 1 for details), it would appear that the passive plume dispersion model in DRIFT Version 2.26 and earlier is appropriate for short averaging times (of the order of 10's of seconds) or moving frame average concentrations as discussed in the Risoe report [12]. This is a consequence of using the same dispersion parameter values as for the near-instantaneous model. To facilitate longer time average predictions (for comparison with the CEA chemical filter measurements) a passive σ_y model based on Draxler [23] has been introduced, with a simple adjustment for averaging time. A selective revalidation of the model against dense and passive datasets has been conducted. The reader is referred to Appendix 1 for details of the changes to the model and the revalidation. The resultant new model is denoted DRIFT Version 2.27.

3.3   REVISED URAHFREP COMPARISONS

With the revised DRIFT model we revisit and extend our comparisons with URAHFREP field trials data.

3.3.1   Trial HF007

We return to the model predictions for Trial HF007. Figure 8 shows the new model concentration predictions using averaging times of 1s and 106s respectively. 106s corresponds to the release duration and is approximately the sampling time for the CEA filter data [16] corrected for arrival and departure time.

DRIFT predicts no generation of positive buoyancy for this trial. The maximum negative buoyancy occurs at around 43m with Ri_*=1.3.

Figure 9 shows model predictions of temperature variation along the centreline, based on 1s time averaging. These predictions are compared with the experimental data points obtained from most positive or most negative temperature deviations as given in Table 4.

3.3.2   Trial HF010

Trial HF010 is a 0.115kg/s release of HF for 178s under slightly unstable, high humidity conditions, with a 10m windspeed of 5.3m/s. Further details are given in Table 1 and Table 3 and the project partners' reports.   Following the procedure outlined in Section 2.2.1 a roughness length of 0.1m has been selected.

Model predictions for concentration are shown in Figure 10.

This release is predicted to generate positive buoyancy. The minimum value of Ri_*=-0.88 occurs at a downwind distance 26m. We have also estimated Hall's lift-off parameter F/u^3W [7] from DRIFT's predictions. This results in $F/u^3W \sim 1.5 \times 10^{-3}$. Both Ri_* and F/u^3W are well within the range where plumes in the wind-tunnel [7] were observed to remain grounded.

Figure 11 shows the model predictions of temperature variation along the centreline, based on 1s time averaging. The experimental data are extracted in the same manner as described for Trial HF007 above.

3.3.3   Trial HF009

Trial HF009 is one of the two trials which mixed isobutane with the HF jet.

Theoretical studies with the HFMIXTURE thermodynamic model indicate that there is sufficient isobutane to cool the cloud to give no rise in temperature above ambient

temperature. There may still be a slight buoyancy increase, but this is much less than would have occurred for a pure HF-moist air mixture.

DRIFT and EJECT dispersion models do not currently allow for the inclusion of isobutane with HF. We shall therefore model the dispersion as a jet of HF, having an initial momentum flux (after depressurisation) equal to the combined momentum fluxes of the HF and isobutane jets. This approach leads to extra dilution during the jet phase, but does not include the cooling or direct dilution resulting from adding isobutane.

Figure 12 shows the DRIFT predictions for trial HF009 modelled this way. Even without the cooling effect of isobutane liquid, DRIFT predicts no generation of positive buoyancy downstream of the momentum jet region for this release. The release appears to behave mostly passively. Of course if we were to model isobutane liquid, then there would be a region over which the plume's density was enhanced.

To model the temperature variation we have run the HFMIXTURE thermodynamic model using the exit and ambient conditions for the trial. The resultant prediction of temperature as a function HF mole fraction (based on HF atoms) is given in Figure 13. It can be seen that the presence of isobutane liquid leads to the prediction of a significantly lower temperature minimum (temperature depression of ~70K) than for the pure HF releases (temperature depression of ~45K). The enhanced temperature drop is due to the extraction of the heat of vaporisation of the isobutane. We note that Table 4 does not include such low temperatures, but this does not preclude such low temperatures occurring closer to the release point. Table 4 indicates a slight warming at 20-25m which is not predicted by the thermodynamic model. This small warming may have resulted from a slight change in ambient temperature during the release.

3.3.4   Trial HF012

Trial HF012 is a 0.125kg/s release of HF for 163s under unstable, high humidity conditions, with a 10m windspeed of only 1.6m/s. This is the most interesting release from the point of view of lift-off. The LIDAR scans indicate that the plume concentration maximum is off the ground at a height of about 20m at 100m. A passive smoke plume shows a similar rise, albeit slightly lower. The clouds are clearly influenced by the strongly convective ambient conditions present. The ambient conditions are changing quite rapidly during this period (becoming more unstable).

Following the procedure outlined in Section 2.2.1 a roughness length of 0.1m has been selected for modelling this trial.

Model predictions are shown in Figure 14. The average concentrations measured by the CEA filters and by the UJF multipoint detectors are clearly significantly less than the model predictions over much of the distance range.

The HF release is predicted to generate positive buoyancy. Positive buoyancy is responsible for enhanced dilution in the model, leading to the downward kink between 20m and 200m. The minimum value of Ri_*=-13.5 occurs at a downwind distance 29m. We estimate the parameter $F/u^3W \sim 0.03$ in this case. Both Ri_* and F/u^3W are within the range where plumes

in the wind-tunnel were observed to partially lift-off giving subsequent downwind ground level concentrations 10-20% of the elevated maximum.

The HF thermodynamics model predicts that the cloud is only positively buoyant up to around 90m distance. Subsequently the cloud is predicted to be denser than air with a maximum $Ri_*=3$ at around 120m. We should stress that these DRIFT model predictions are based on the cloud remaining grounded.

As discussed by Risoe [12] the problem with Trial HF012 is whether any of the observed lift-off is attributable to HF thermodynamic behaviour of the cloud. The DRIFT model predictions together with lift-parameters clearly indicate the potential for some lift-off to have occurred due to HF thermodynamics, in the absence of ambient convection. Clearly, in the case of HF012, ambient convection has the capability to dominate. The Risoe approach of surface layer scaling [12] seems to offer the most promise of finding any small residual HF buoyancy effect. These studies indicate that if there is an effect, it is small compared with ambient convection.

4 Predictions for Other Release and Ambient Conditions

In Section 3 we made comparisons of model predictions with URAHFREP field trials data. We found that in most cases the models indicate the release rates are insufficient to show any significant effect of HF thermodynamics on concentration. This is borne out by the experimental observations. The only exception is possibly Trial HF012 which the model indicates may partially lift-off due to HF thermodynamic effects (based on the predicted lift-off parameter). The strongly convective ambient conditions during this trial may have masked this effect. Current models do not account for the effect of convective ambient conditions on lift-off.

In the absence of strong evidence of HF induced lift-off in these medium scale field trials, it is instructive to use the dispersion models to investigate the conditions under which HF induced lift-off may occur. In particular, there is an interest in the effect of going to larger release sizes and to stable atmospheric conditions.

4.1 LARGER SCALE RELEASES

As a base case we shall consider dispersion under the ambient conditions reported for trial HF010 (see Table 3). Trial HF010 is under effectively neutral atmospheric conditions. The model predictions based on the 0.1kg/s release indicate that no lift-off would be expected based on the Ri_* and F/u^3W lift-off parameters. Let us consider the effect of increasing the release rate on the Ri_* value.

We shall scale the mass flux according to the square of the exit diameter. Other than the exit diameter and mass flux the release conditions are taken to be unchanged from those of Trial HF010. Table 5 shows the predicted minimum value of Ri_* and the distance at which it occurs as a function of HF mass flux. Short (1s) time averaging has been used in the model. The results are illustrated in Figure 16.

Exit diameter (mm)	HF mass flux (kg/s)	min Ri_*	distance to min Ri* (m)
2.5	0.113	-0.88	26
8	1.16	-2.32	66
25	11.3	-5.84	203
50	45.2	-10.2	388
100	180.8	-18.9	725

Table 5. Predicted minima of Ri_* and the distances at which they occur as function of HF mass flux.

Not surprisingly, scaling up the release rate increases the absolute magnitude of the minimum Ri_* value for fixed conditions, i.e. gravitational effects become more important for the larger scale release.

Using the lift-off behaviour in wind-tunnel studies [7,11] as a guide to the possible lift-off behaviour, the centreline maximum concentration may just be starting to rise above ground for the 1kg/s release. At 45kg/s the ground level concentration may be 10-20% of the concentration maximum.

4.2   ATMOSPHERIC CONDITIONS

Wind tunnel studies show the large effect of ambient windspeed on lift-off in neutrally stable atmospheric conditions. Low windspeeds greatly enhance the chances of lift-off . Low windspeeds during daytime insolation lead to unstable atmospheric conditions which, as shown by the URAHFREP field trials, may mask the buoyancy effects of HF thermodynamics on the plume. Conversely low windspeed stable conditions, as occurring during a clear night, may enhance the buoyancy effects due to the HF thermodynamics.

To illustrate the sensitivity of model predictions to atmospheric stability we consider a 1kg/s HF release under different atmospheric stabilities as classified using Pasquill categories. The 1kg/s release rate is assumed to arise from the HF010 exit conditions with an exit diameter of 8mm and release height of 1.2m. A 10m windspeed of 2m/s is assumed throughout, with a surface roughness length of 0.1m. Relative humidity is set at 90% and the ambient temperature set to 10°C. The model results for Ri_* are summarised in Table 6.

Pasquill Stability	min Ri_*	distance to min Ri_* (m)	distance to Ri_*=-10 (m)
A	-18	68	52
B	-20	78	56
C	-24	90	61
D	-29	112	66
E	-43	134	75
F	<-70	113	88

Table 6. Predicted minima of Ri_* and the distances at which they occur as function of atmospheric stability for a 1kg/s release, 90% relative humidity with a 2m/s windspeed at 10m. Also shown are the distances to Ri_*=-10.

Table 6 shows only a small sensitivity of the minimum Ri_* value to stability when atmospheric conditions are unstable. The minimum Ri_* value is much more sensitive to stable conditions. This reflects the decrease in dilution rate for the cloud due to strong suppression of vertical mixing. The validity of the Ri_* prediction for stable low windspeed conditions is subject to the considerable uncertainties in dense gas dispersion modelling of this regime.

For the reasons mentioned above, the wind-tunnel studies for neutral atmospheric stability are not directly applicable to lift-off under non-neutral stability.

5   Conclusions

It is important to be clear about the basis of our modelling in this study. The results are mainly dependent on the DRIFT dispersion model, which includes enhanced dilution due to positive buoyancy, but not lift-off. Lift-off behaviour has been inferred from the model predictions of lift-off parameters Ri_* and $F/u^3 W$ and the observations in the URAHFREP wind-tunnel studies at these parameter values. For non-buoyancy conserving plumes, such as HF in moist air, it is argued that the adopted approach may be most suited to determining *whether* lift-off occurs, rather than in predicting the subsequent plume rise.

The main conclusion to be drawn from our study is that the model predictions appear to be consistent with the observed (non) lift-off behaviour (excluding trial HF012) of the URAHFREP field trials. For trial HF012, model predictions are that sufficient buoyancy is generated due to HF thermodynamics for partial lift-off to occur. However, its seems likely based on the analysis of [12] that the strongly convective ambient conditions occurring during this trial probably dominate any influence of HF.

Excepting trial HF012, there is very little difference in predictions of concentrations between model runs incorporating HF thermodynamics and runs assuming passive behaviour. This indicates that for the prevailing atmospheric conditions, except for the dense jet phase near to the source, the releases are too small to show significant gravitational effects.

Additional calculations show how increasing the size of release or going to more stable atmospheric conditions may enhance the chances of lift-off. Our approach, based on the observed wind-tunnel behaviour, may overstate lift-off in unstable conditions. This is because downdrafts in unstable conditions may lead to clouds remaining ground based, which otherwise would be expected to lift-off. Conversely, lift-off may be understated in stable conditions. This is because plumes which, due to the vertical mixing, do not lift-off under neutral conditions, may lift-off under stable conditions where this vertical mixing is suppressed.

Our comparisons with Field Trials data highlight the fact that models do not predict the 'dilution' resulting from low frequency meander of the plume due to wind direction changes or ambient convective motion in unstable conditions. Whilst this might be reasonable if one is interested in short time effects, it may lead to significant pessimism for situations which require a longer time exposure.

Because of the importance of passive dispersion in the URAHFREP trials, the lateral spreading rate in DRIFT's passive dispersion model has been reviewed and as a consequence revised. A simple 'model' for the effect of averaging time has also been introduced. For short averaging time the model reverts to the original 'instantaneous' formalism. The new passive approach is arguably more soundly based. However, some concerns remain regarding the adequacy of the lateral spread and averaging time models. A fuller validation study may be required to fully endorse the lateral spread model, and consideration should also be given to incorporating more advanced averaging time models utilising the recently improved understanding of concentration fluctuations [25].

6   Acknowledgements

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8   Figures
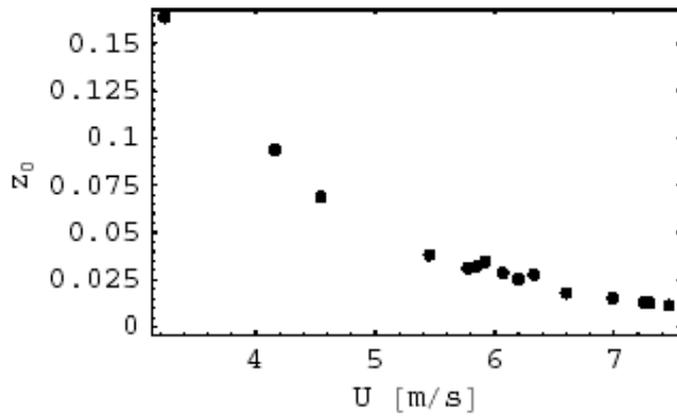
Figure 1. Observed variation of roughness length, z_0 (m) with windspeed. (reproduced from Risoe report R 1212(EN).
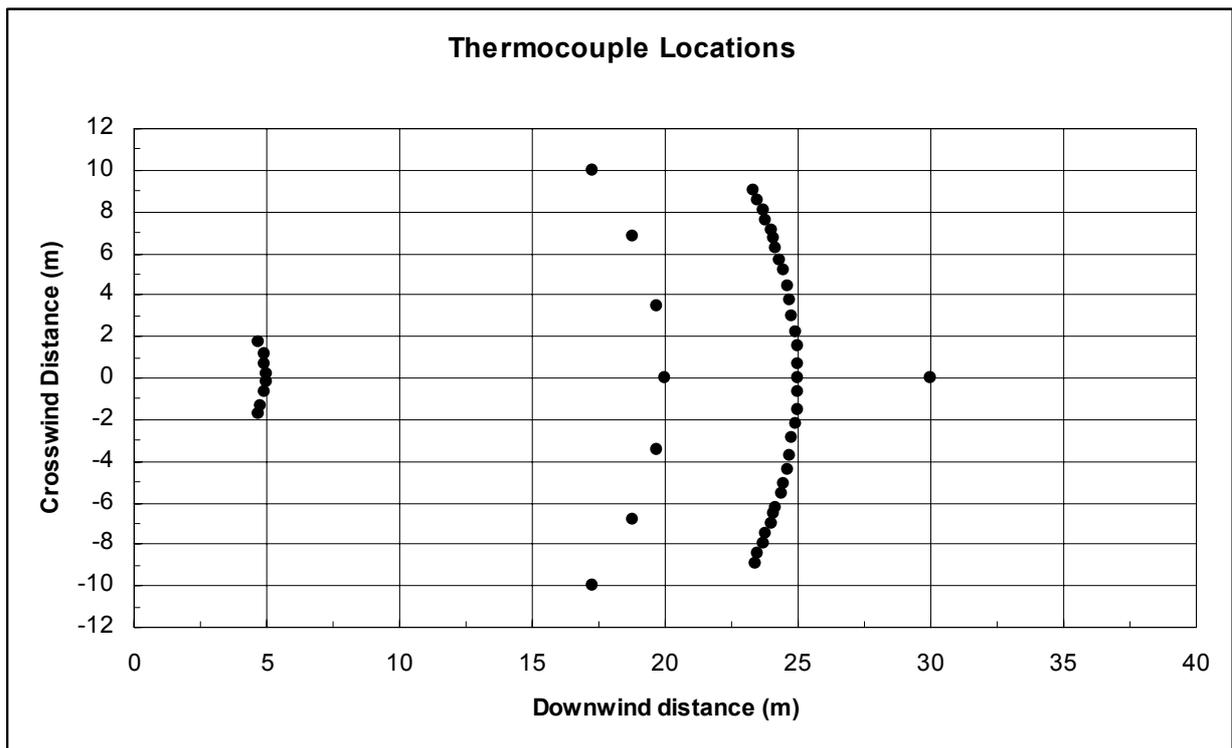
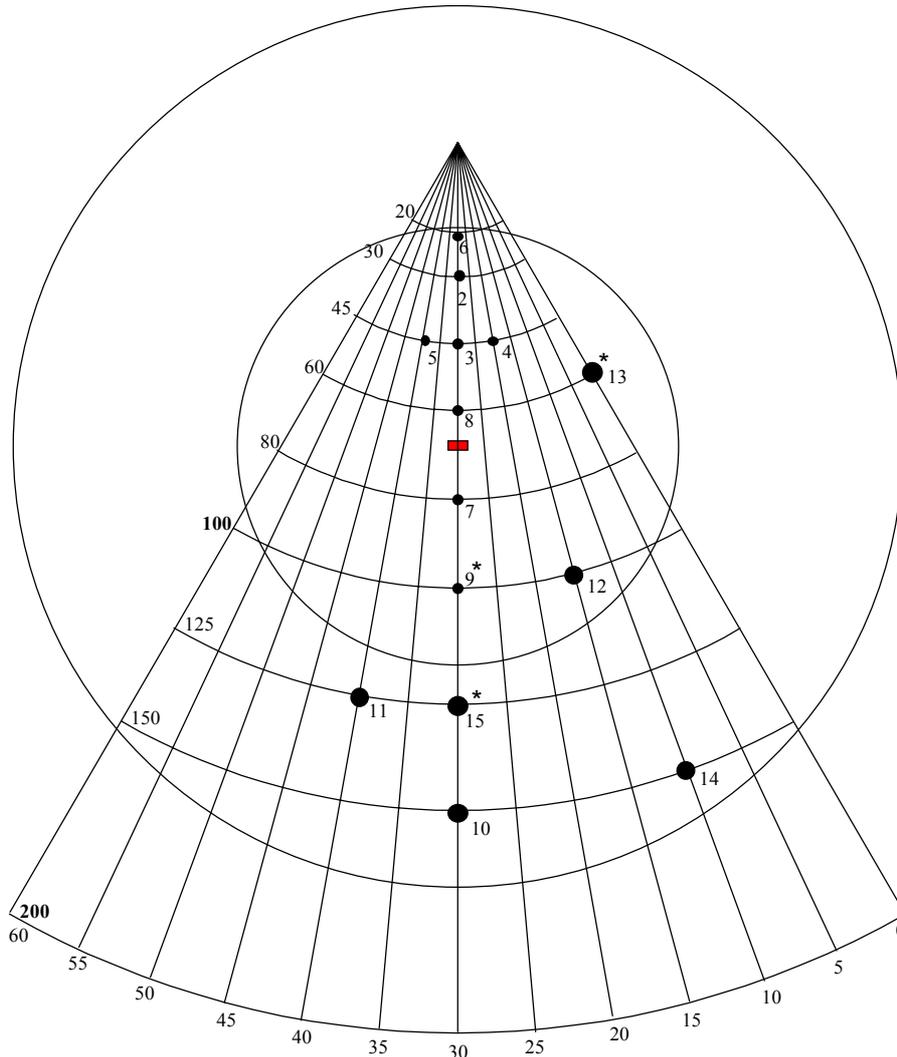**Figure 2. Thermocouple locations relative to source at (0,0).**

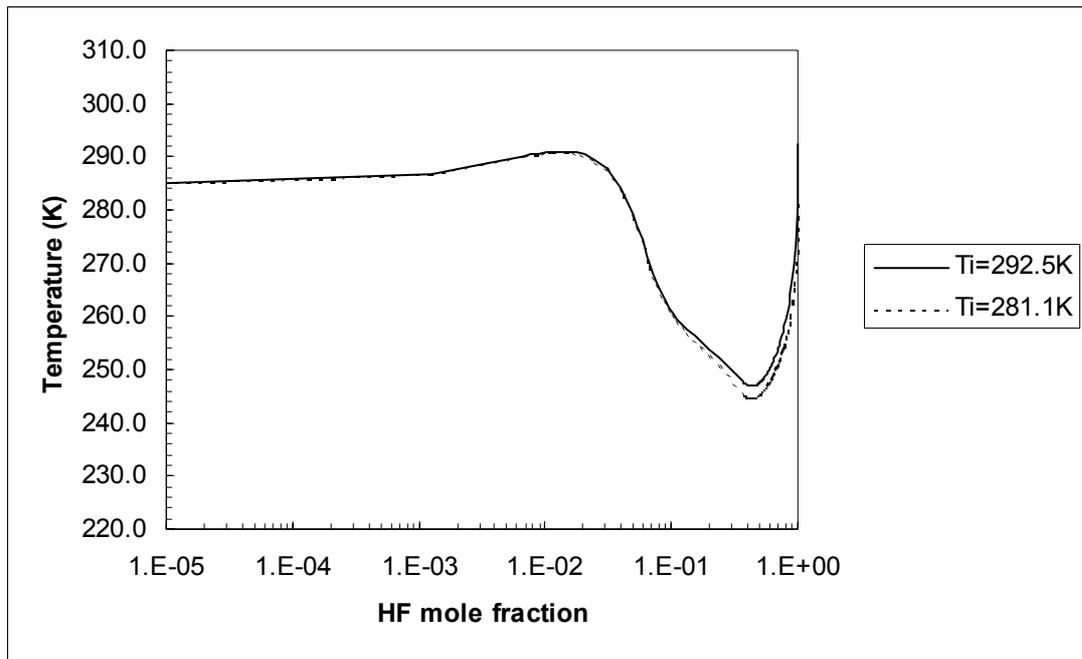**Figure 3. Near-Field Concentration Measuring Locations**

Figure 4. HFMIXTURE prediction of the effect of initial liquid temperature on mixture temperature as a function of HF mole fraction (based on Mw=20) for conditions appropriate for Trial HF012
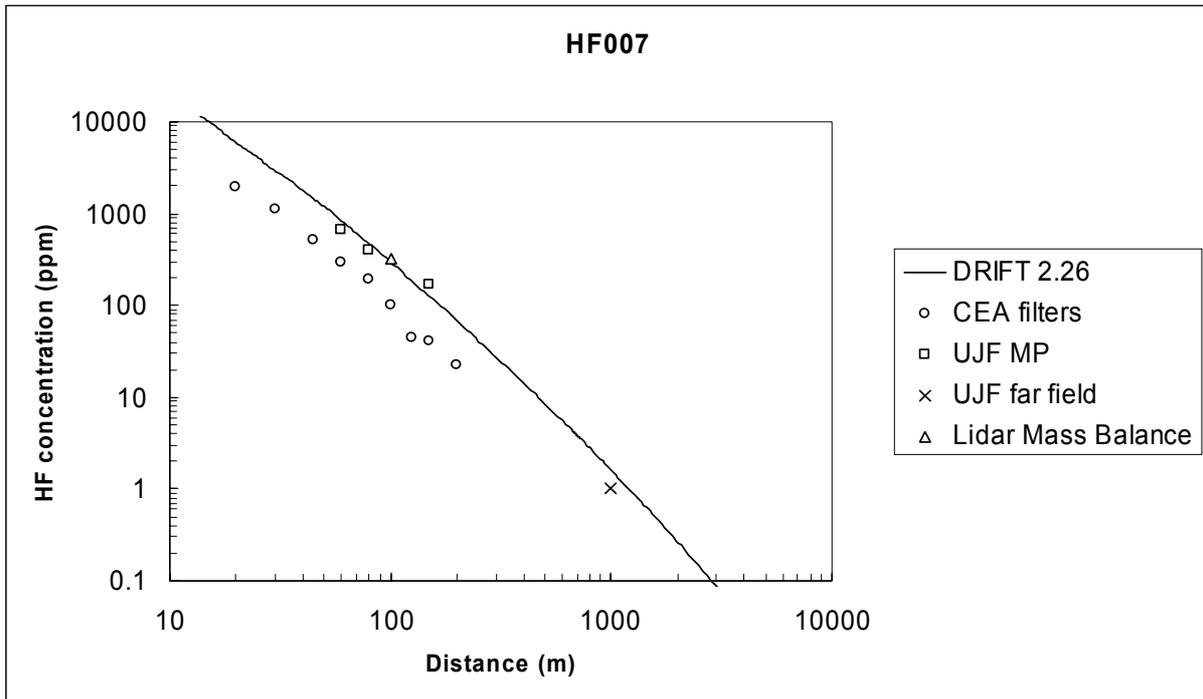
Figure 5. DRIFT 2.26 ground level centreline concentration predictions for Trial HF007.
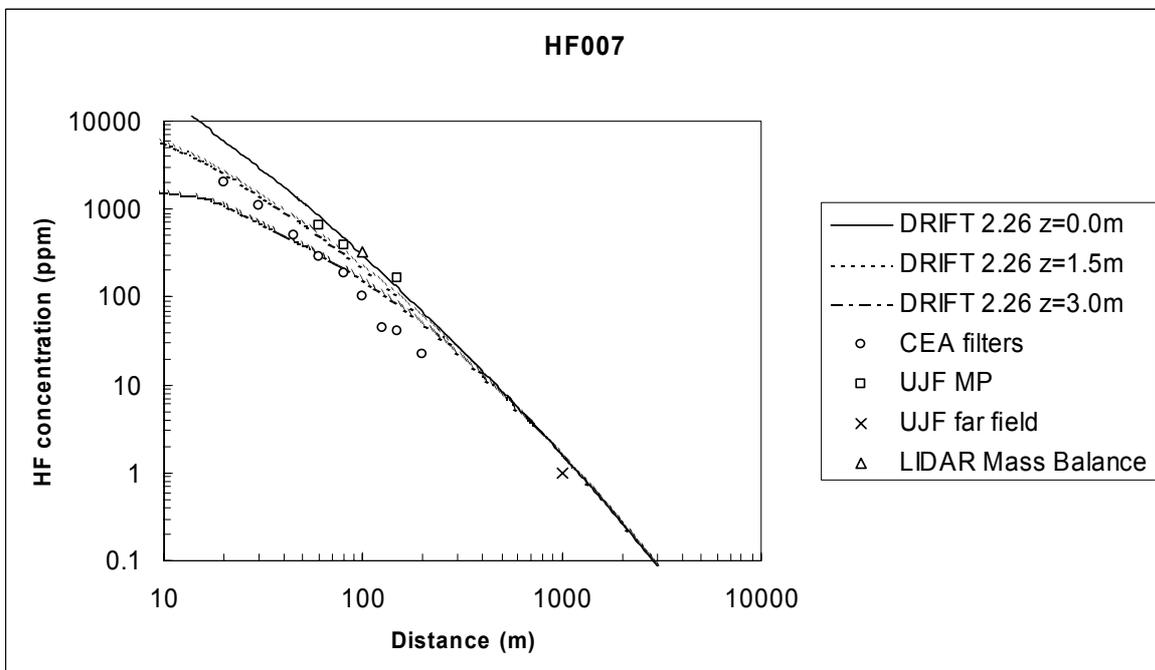
Figure 6. DRIFT 2.26 concentration predictions as a function of receptor height for Trial HF007.
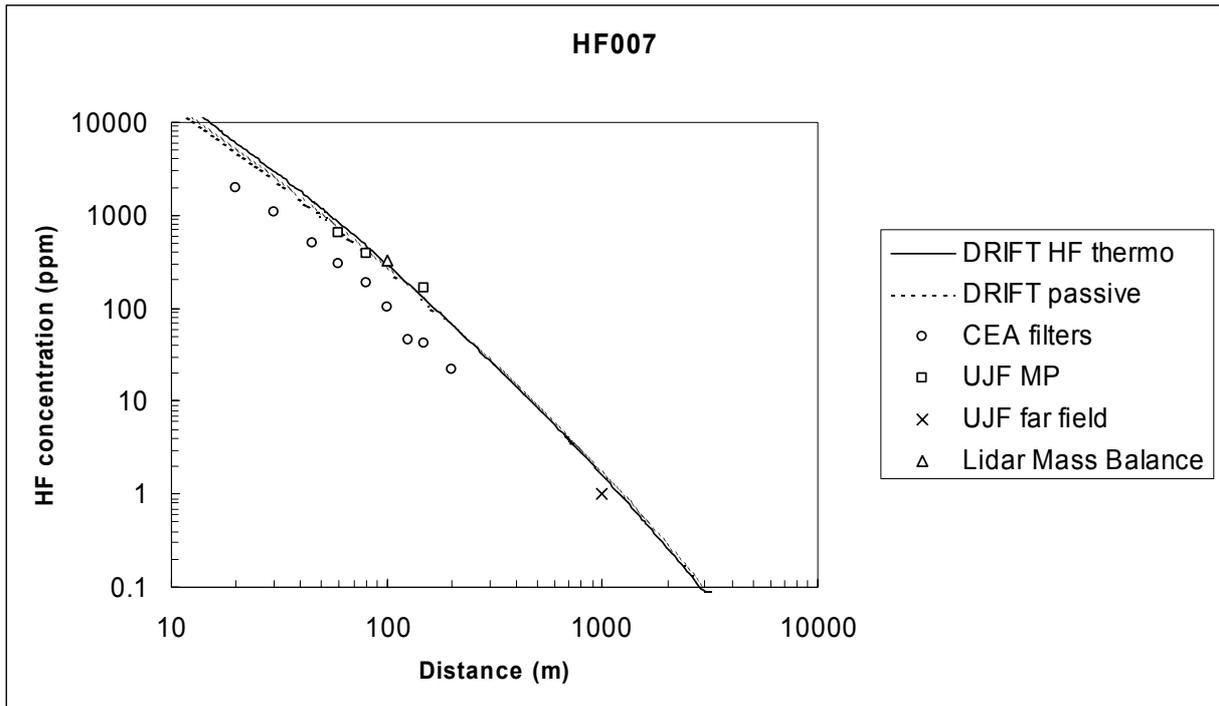
Figure 7. DRIFT 2.26 predictions for Trial HF007 using HF thermodynamics compared with DRIFT predictions using a passive source.
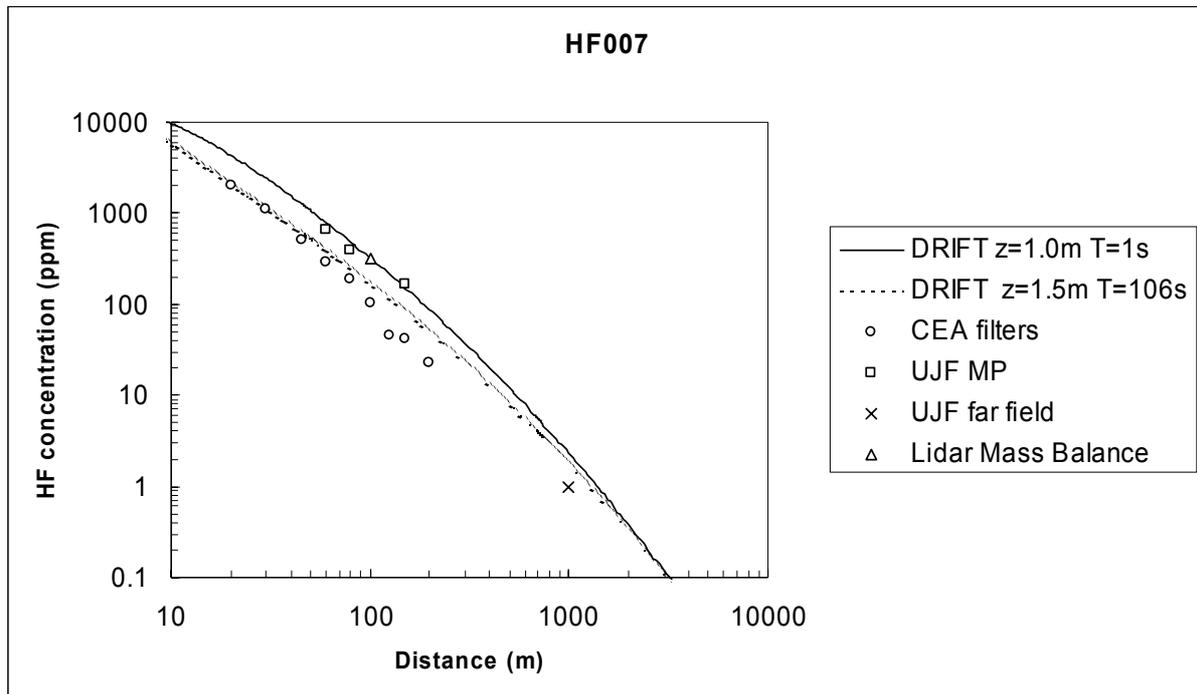
HF007

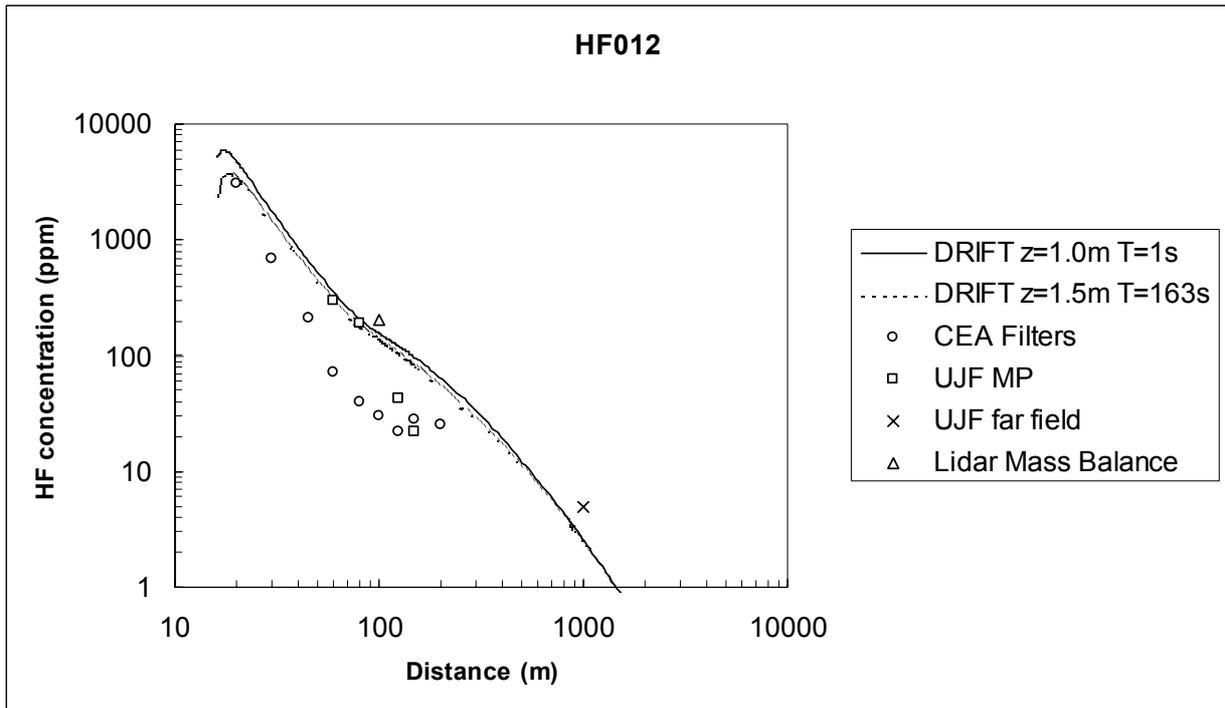**Figure 8. DRIFT 2.27 predictions forTrial HF007. z indicates receptor height and T the model averaging time.**

HF007
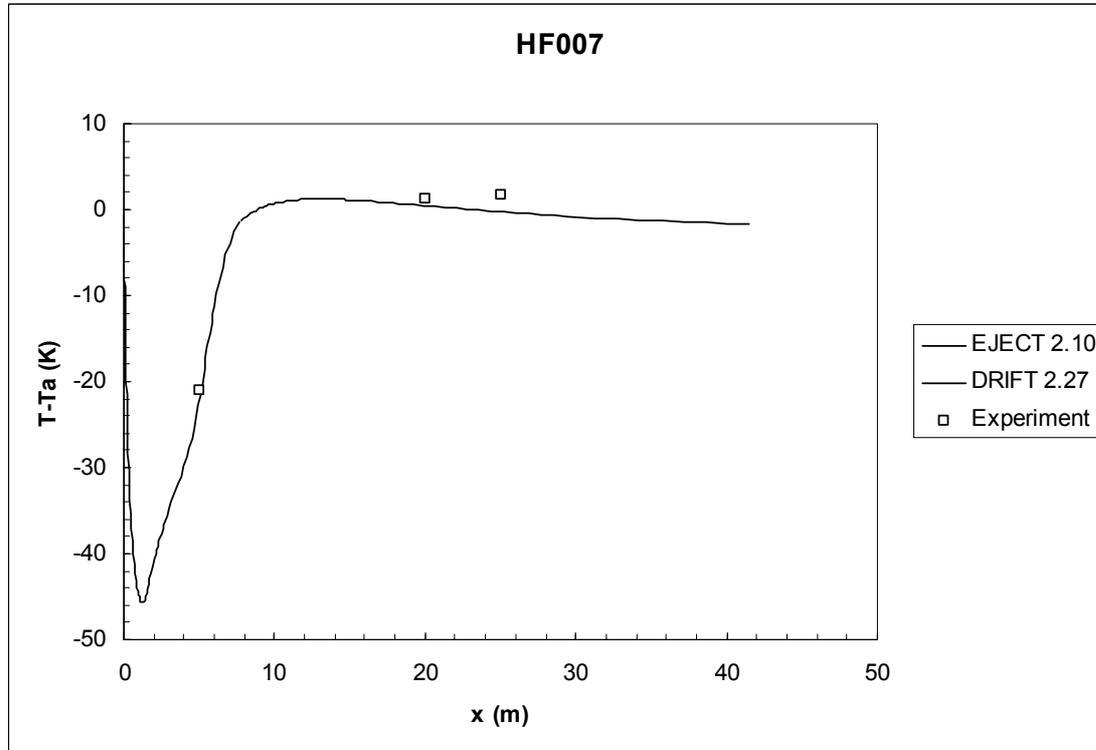
Figure 9. EJECT and DRIFT predictions for maximum temperature difference from ambient temperature.
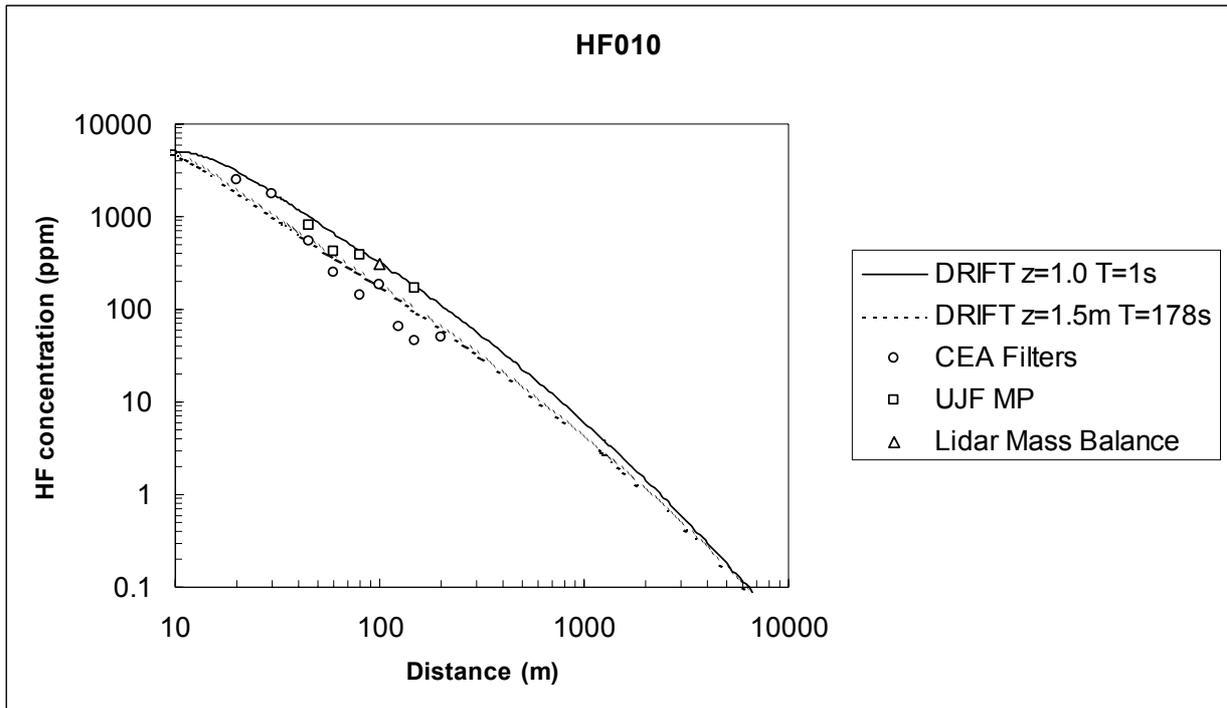
HF010

Figure 10. DRIFT 2.27 predictions for Trial HF010. z indicates receptor height and T the model averaging time.

HF010
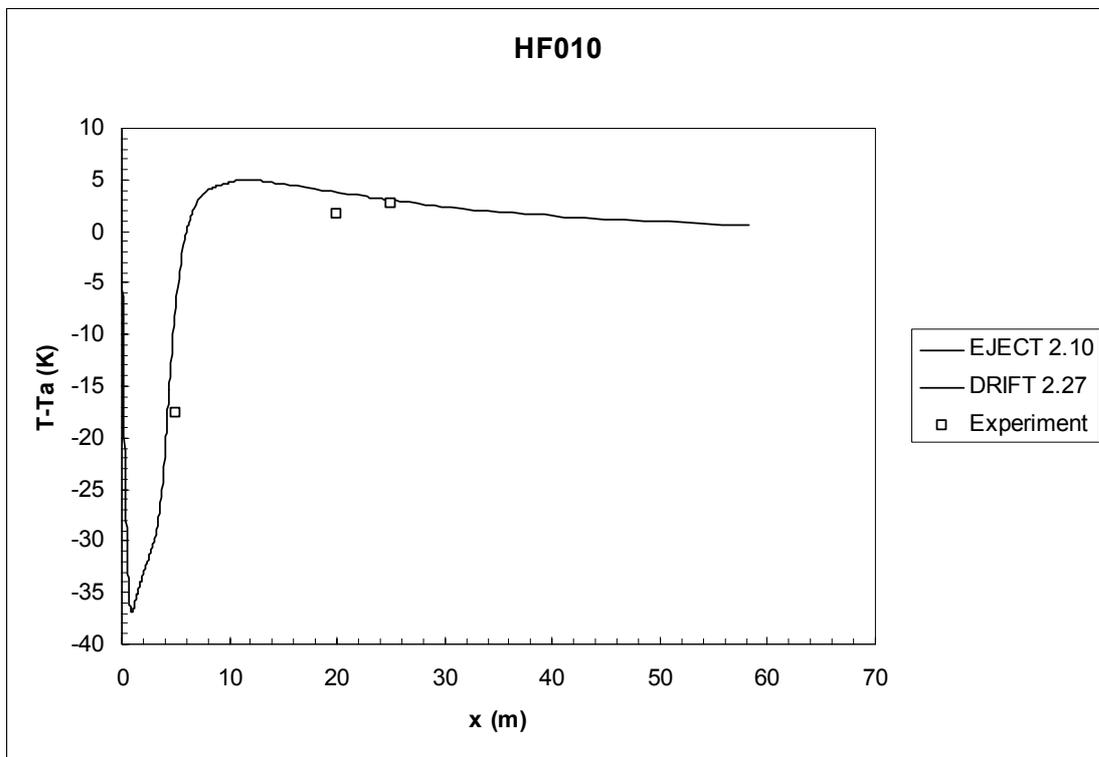
Figure 11. EJECT and DRIFT predictions for maximum temperature difference from ambient temperature.
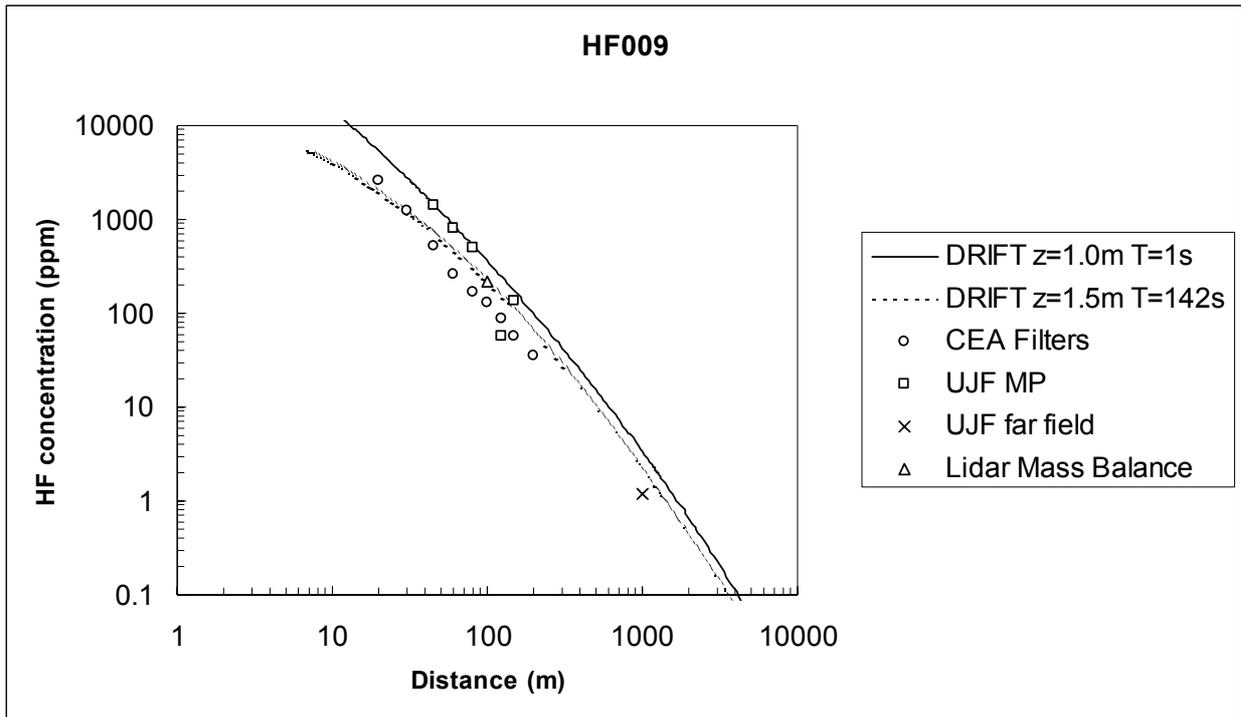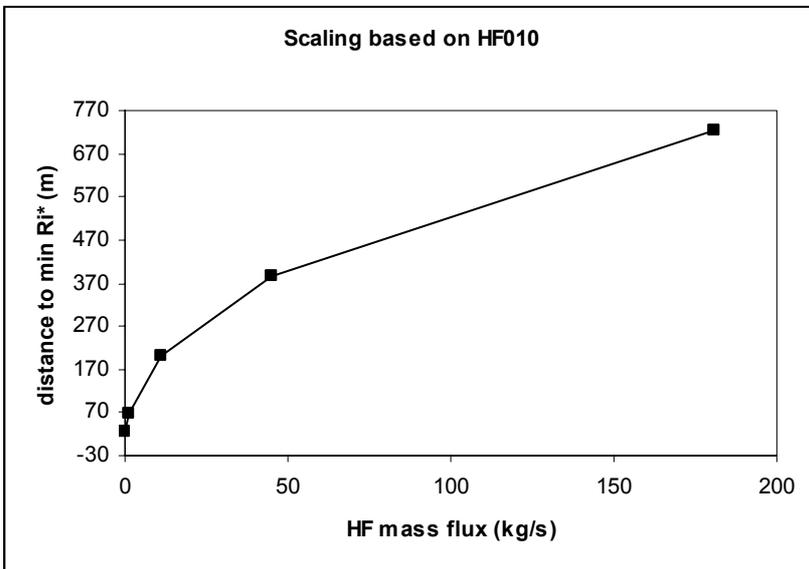
Figure 12. DRIFT 2.27 predictions for Trial HF009. z indicates receptor height and T the model averaging time.
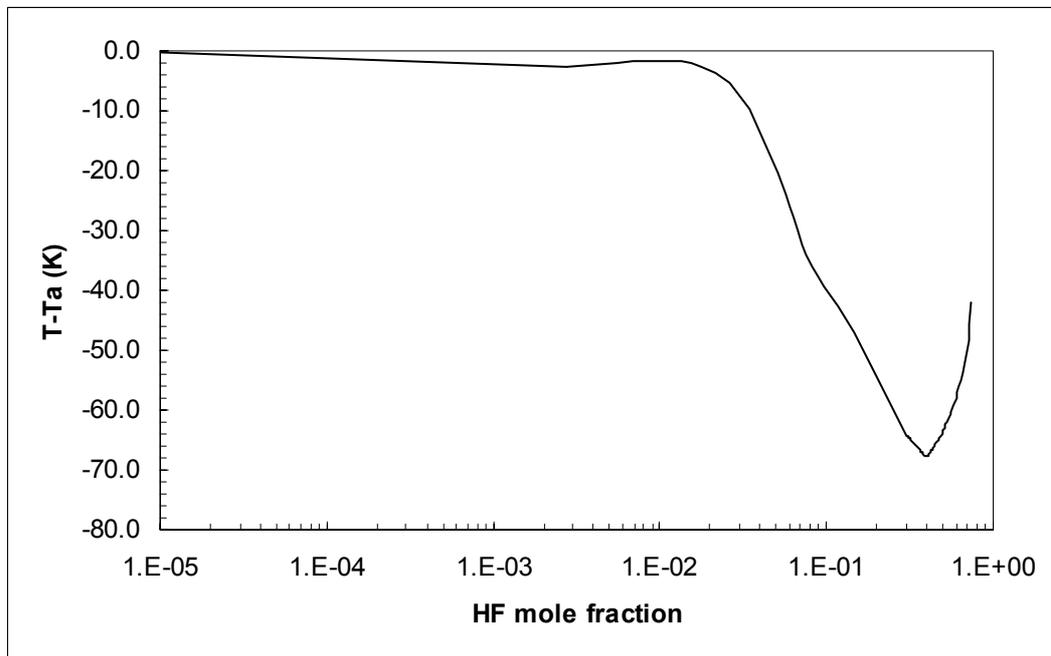
Figure 13. HFMIXTURE prediction of temperature difference from ambient of mixing liquid HF and isobutane under the conditions of Trial HF009.

Figure 14. DRIFT 2.27 predictions for Trial HF012. z indicates receptor height and T the model averaging time.
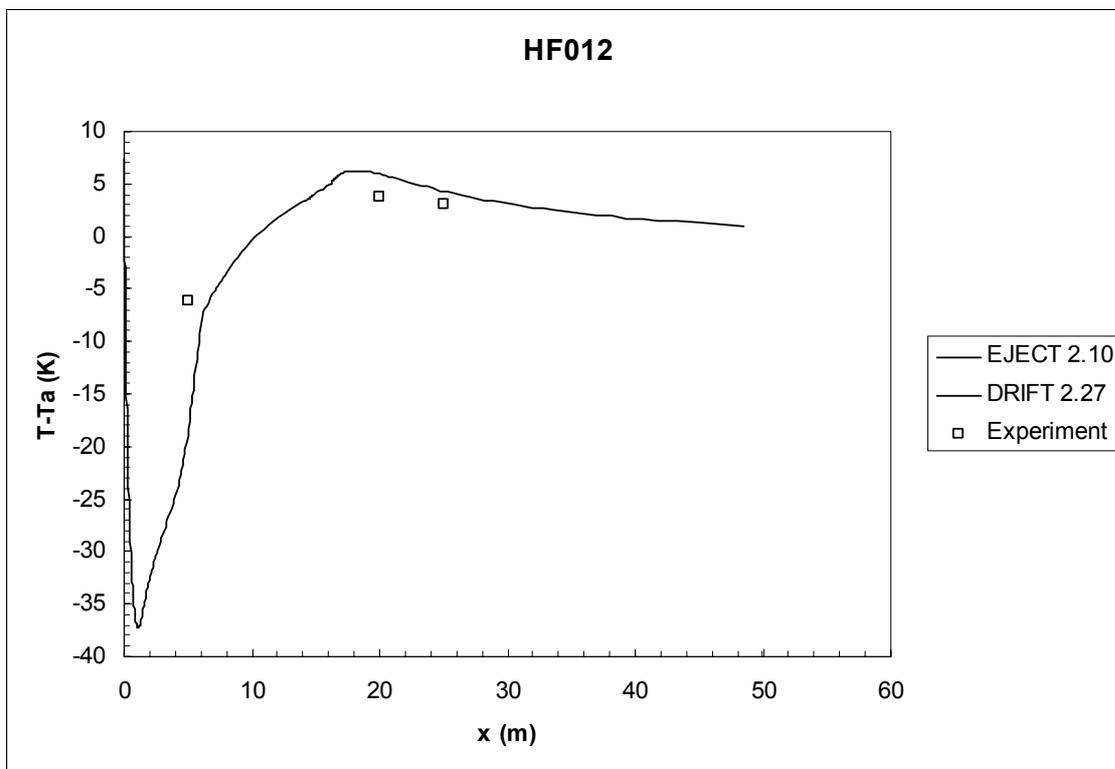
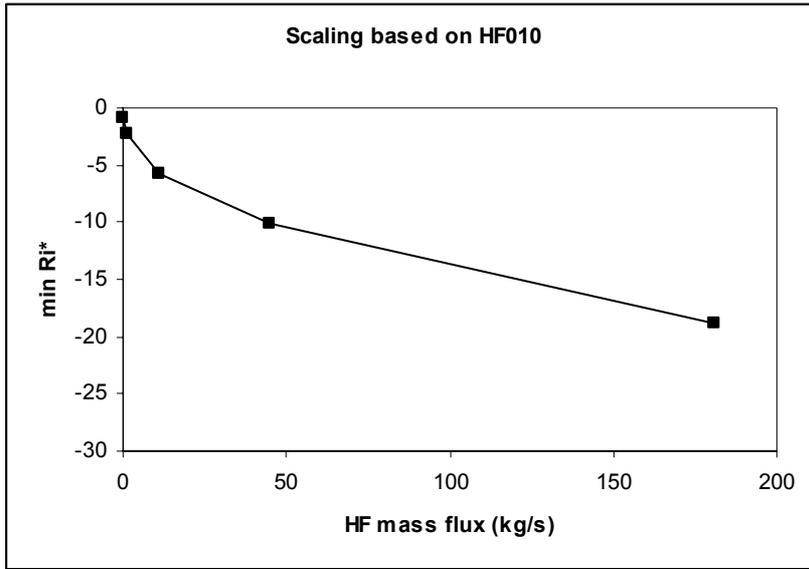**Figure 15. EJECT and DRIFT predictions for maximum temperature difference from ambient temperature.**

Figure 16. Predicted scaling with HF mass flux of the minimum Ri* and the distance at which it occurs. Conditions based on URAHFREP Trial HF010.

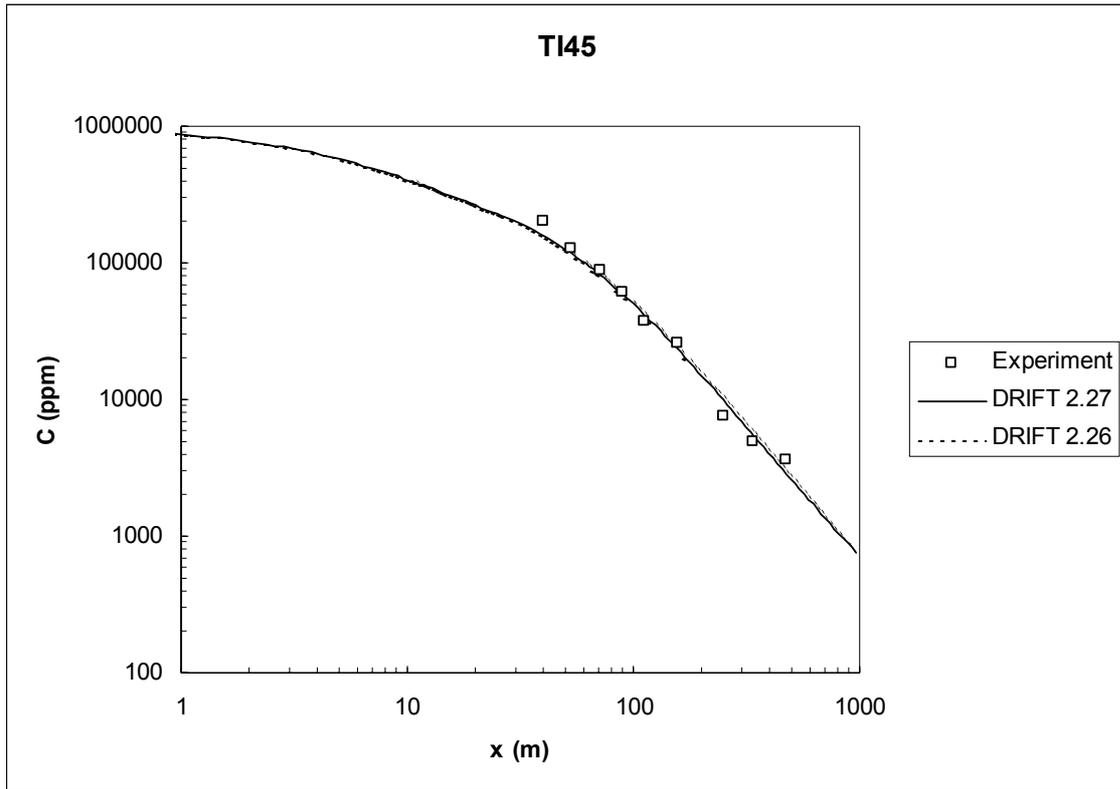**Figure 17. DRIFT predictions for Thorney Island Trial 45. Note DRIFT 2.26 was tuned against this data.**
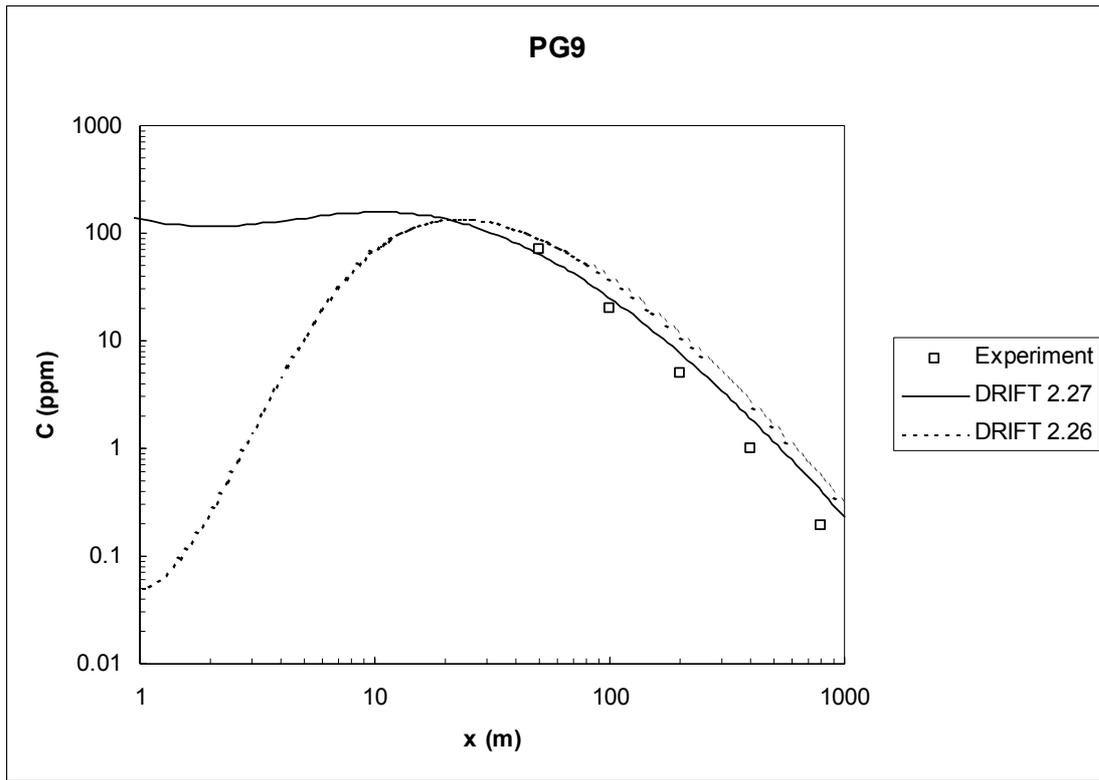
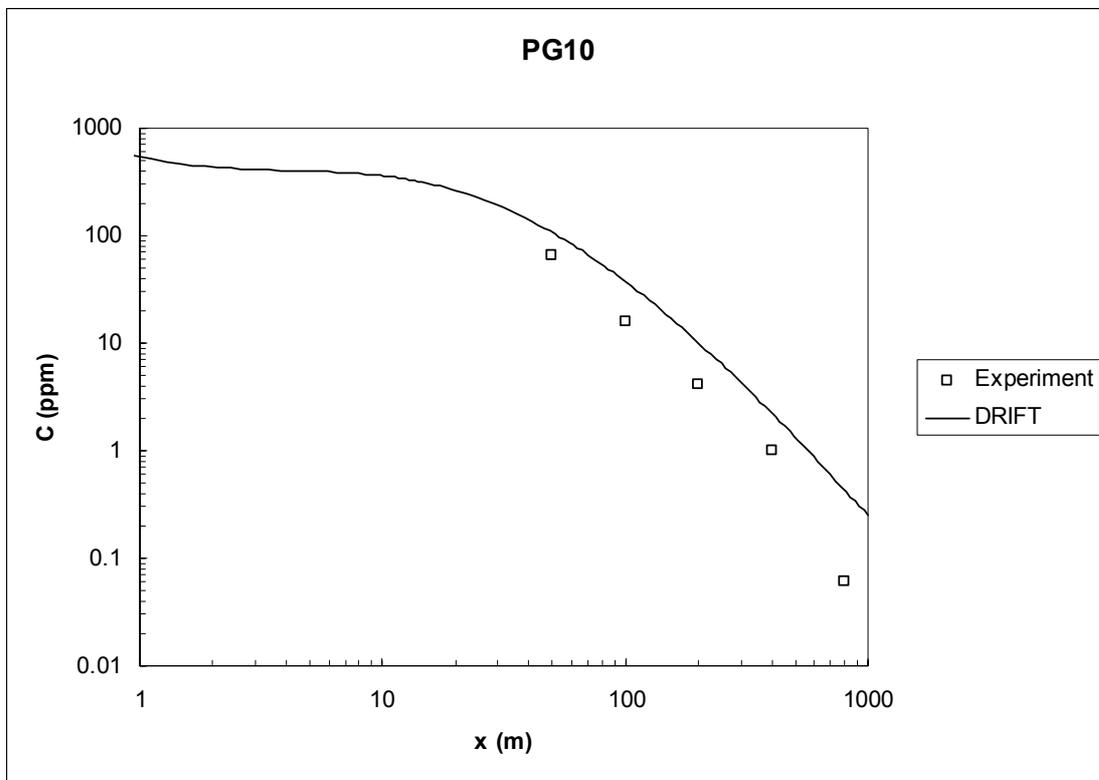**Figure 18. DRIFT predictions for Prairie Grass Trial PG9.**

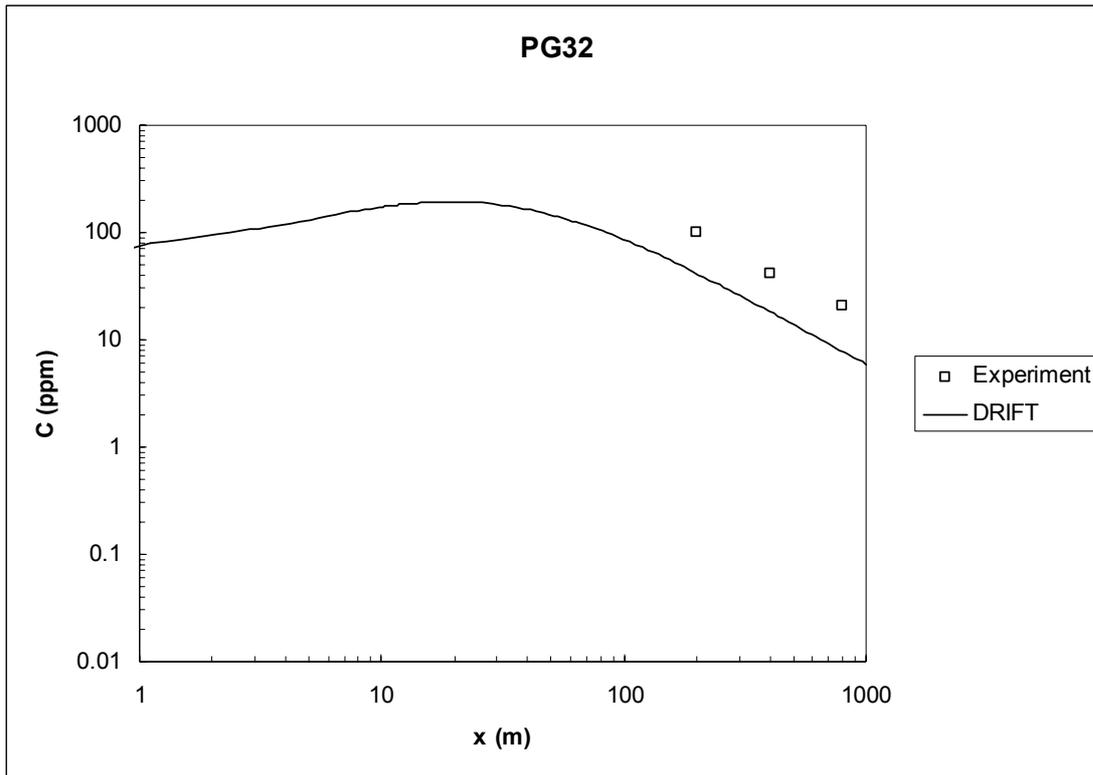**Figure 19. DRIFT 2.27 predictions for Prairie Grass Trial PG10.**

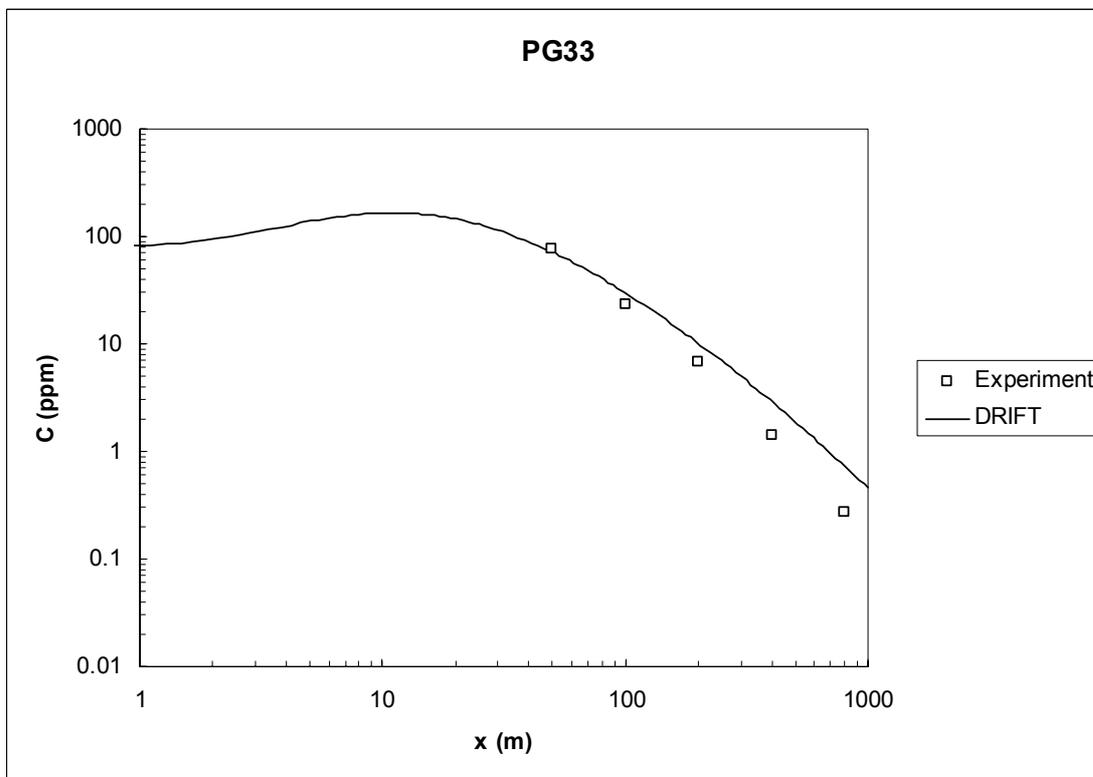**Figure 20. DRIFT 2.27 predictions for Prairie Grass Trial PG32.**

Figure 21. DRIFT 2.27 predictions for Prairie Grass Trial PG33.
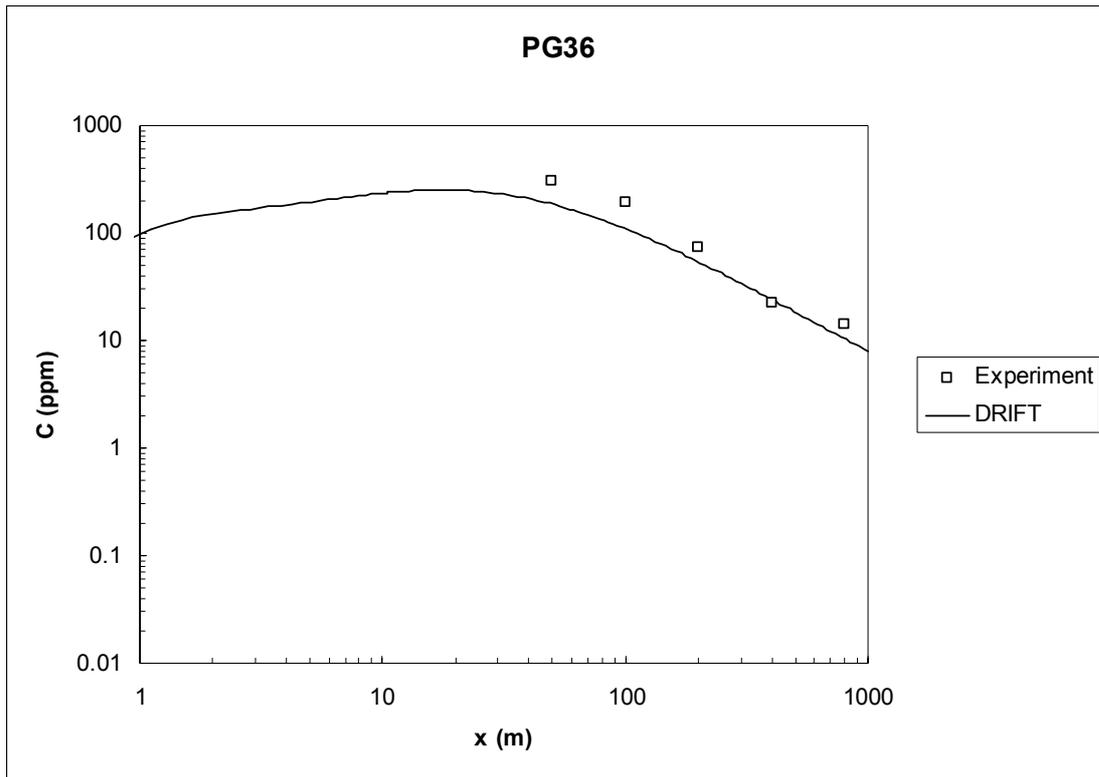
Figure 22. DRIFT 2.27 predictions for Prairie Grass Trial PG36.

Appendix 1.   Review and Revision of DRIFT's Passive Plume Model

Our comparison of DRIFT predictions with concentration measurements for URAHFREP Trial HF007 indicate that DRIFT is in closest agreement with the peak or short time averaged data (UJF and LIDAR mass balance). A cursory comparison with the other URAHFREP trials indicates that this is generally the case. Is this what we should expect from DRIFT's passive model?

The time averaging in DRIFT is wholly implicit, and is based on the entrainment parameter values adopted by the model. Refs. [10,18] indicate that, in the passive limit, the appropriate time averaging is roughly the 15min sampling time discussed by Businger et al [21]. Based on this, one might (naively) expect that DRIFT's predictions should be lower than the peak or short time averaged values. This does not appear to be the case.

Perhaps not surprisingly, most of DRIFT's validation studies relate to datasets dominated by the dense gas phase [22]. DRIFT's passive model has received little or no validation attention. Given that most URAHFREP releases seem to be dominated by passive behaviour, it is now timely, possibly even overdue, to review DRIFT's passive plume model.

A1.1   VERTICAL SPREAD

Vertical spreading in the passive plume model is obtained from solutions of the vertical diffusion equation, using power law approximations for windspeed and diffusivity changes with height. The profiles are based on those of Businger [21]. The theoretical basis for the approach seems justified and the method includes the effects of surface roughness and atmospheric stability in accord with atmospheric similarity theory.

A1.2   LATERAL SPREAD

The main influence of time averaging is on the lateral standard deviation σ_y. DRIFT's passive plume model for σ_y is

$$\frac{d\sigma_y}{dx} = 0.3 \frac{\sigma_v}{\overline{u}} \tag{10}$$

where σ_v is the root mean square lateral velocity fluctuation and $\overline{u}$ is the plume advection velocity. DRIFT assumes $\sigma_v = 2.0 u_*$ for all atmospheric stabilities.

Exactly the same spreading formula is used by DRIFT for continuous and instantaneous releases. This must be highly questionable, especially in the near field. There are theoretical reasons why the spreading rate for dispersion from a maintained continuous source in the near field differs from the spreading rate for a puff release. The 0.3 proportionality constant comes from experiments on puff releases of lycopodium spores [17]. For plumes it is widely accepted that

$$\frac{d\sigma_y}{dx} \rightarrow \frac{\sigma_v}{\overline{u}} \qquad\qquad (11)$$

in the near field [17]. It would seem more appropriate for the passive plume model to use the model of Draxler [23]:

$$\sigma_y = \frac{\sigma_v}{\overline{u}} \frac{x}{1 + 0.9(x/\overline{u}t_i)^{1/2}} \qquad\qquad (12)$$

which has more appropriate asymptotic limits. Draxler suggests a value of $t_i=300$s for ground level releases. In the near field, using the same $\sigma_v/\overline{u}$, the Draxler will give a dilution rate about 3 times larger than the instantaneous model's 0.3 factor. It seems to us that for passive plumes the Draxler formulation is more appropriate and that this should be adopted by DRIFT.

The explicit x dependence in the Draxler formula makes it fit somewhat awkwardly into DRIFT which attempts to avoid such global dependencies and work with local rates of change. The Draxler formula may be incorporated into DRIFT by solving for x from the current cloud σ_y and using the differential of equation (12) with respect x to give the rate of passive spread. As previously, the spreading rate used by DRIFT is chosen to be the maximum of passive and the other spread mechanisms (e.g. gravity spreading).

The adequacy of the $\sigma_v = 2.0u_*$ relation is open to question, particularly under unstable conditions. The factor of approximately 2 seems quite well established for neutral conditions over flat terrain [24]. In unstable conditions convection can contribute significantly to σ_v. In very stable conditions variability in wind direction can lead to enhanced σ_v above that of the (low) mechanical turbulence characterised by u_*. These effects are currently ignored by DRIFT.

A1.3   LATERAL PROFILE SHAPE

DRIFT makes a continuous transition between the dense and passive dispersion regimes. The lateral concentration distribution is controlled by the shape parameter w in:

$$F_h = \exp\left[-\left(\frac{y}{b}\right)^w\right] \tag{13}$$

DRIFT models w according to

$$w = 2 + (w_T - 2)\frac{Ri_h}{Ri_T} \tag{14}$$

where, the 'horizontal' Richardson number, $Ri_h = \dfrac{g\Delta\rho H}{\rho_a \sigma_v^2}$, is a measure of the erosion of the uniform profile by lateral velocity fluctuations. DRIFT 2.26 and earlier adopt w_T=50 and Ri_T=1. The choice of these parameter values means that even when Ri_h=0.1 (ie lateral velocity fluctuations contain 10 times the cloud's gravitational potential energy) w=6.8, which still gives a fairly uniform profile. In our opinion there is little or no evidence to support holding on to uniform lateral profiles for so long (if at all). It would seem to be more appropriate to chose w_T=3, so that when Ri_h=0.1, w=2.3, which is much closer to Gaussian. According to equation (14) the profile would then be close to uniform when Ri_h=10, i.e. when gravitation potential energy dominates the lateral ambient velocity fluctuations. This behaviour in our opinion seems more reasonable.

Altering the w transition in this way requires also a slight change to the modelling of top entrainment dense to passive transition in DRIFT, which has previously depended explicitly on w. It is suggested that the edge entrainment velocity , u_E is simply based on the maximum of the gravity and passive edge entrainment velocities:

$$u_E(adv) = \max(u_E(grav), u_E(pass)) \tag{15}$$

with

$$u_E(grav) = \alpha_E U_f \tag{16}$$

and

$$u_E(pass) = \frac{d\sigma_y}{dx}\overline{u}\left[\frac{3\Gamma(1+1/w)^3}{\Gamma(1+3/w)}\right]^{1/2} \tag{17}$$

where U_f is the gravitational spread velocity (value unaltered from DRIFT 2.26), α_E an edge entrainment coefficient for gravity spread (value unaltered from DRIFT 2.26) and $\Gamma(x)$ is the Gamma function .

It is expected that making the above changes should have little effect in the dense gas limit, but should give a sounder basis in the passive limit. The arbiter of such changes should, of course, be validation against suitable experimental data. We shall consider this validation in Section A1.6.

A1.4   TIME AVERAGING

We have still not really solved the time averaging problem. What time averages is DRIFT predicting in the passive limit?

One might expect the appropriate time average is the sampling time for σ_v. Using the model $\sigma_v = 2.0 u_*$ seems to imply an averaging time sufficient for the plume to dilute according to mechanical turbulence. This would include the higher frequency fluctuations which can dilute the plume, but we suspect does not include lower frequency fluctuations due to for example convective turbulence and lower frequency changes in wind direction which we understand [17] are usually filtered out from meteorological measurements of σ_v.

The above is simply a statement that the model cannot deal with larger scale convective or meandering motion. It does not tell us what the time averaging period should be. Indeed there may be no such time universally valid at all positions in the plume. In the absence of implementing more sophisticated models for concentration fluctuation and plume meander [25] we shall simply assume that using $\sigma_v = 2.0 u_*$ is equivalent to an averaging time of a few minutes (say 10min). The effect of low frequency plume meander or large scale convective motion are not included in this averaging.

We shall employ the oft used $\tau^{0.2}$ scaling [26] of concentration with averaging time τ to predict concentrations at different averaging times. This is subject to a maximum concentration equal to the instantaneous plume concentration as predicted by the $0.3\,\sigma_v$ model, i.e. short time averaging will still use the $0.3\,\sigma_v$ model.

This crude approach to time averaging will be adopted for our subsequent model comparisons.

A1.5   DRIFT VERSION 2.27

A new version of DRIFT incorporating the above changes has been produced. This version is denoted as DRIFT 2.27.

During the course of producing DRIFT 2.27 a coding error was noticed for the passive lateral spread in Version 2.26. The result of the error was that the lateral spread was about 20% higher than indicated by equation (10), which to some extent compensates for some of the under dilution of the $0.3\,\sigma_v$ model.

A1.6   DRIFT REVALIDATION

With the above changes made to DRIFT it is necessary to check that the existing published validation of the model is still appropriate and that the new passive model performs adequately.

We do not expect the changes to have a marked effect on the dense gas limit, but we should check this since we have altered the top entrainment/passive transition. It would be too much work to check all the previous validation studies under the current project. Instead we choose some representative trials to see if our expectations are correct. In addition we compare the model against Prairie Grass passive dispersion trials data from Hanna's Modelers Data Archive (MDA) [27].

A1.6.1   Dense Gas Datasets

Figure 17 shows the predictions of DRIFT 2.27 compared with DRIFT 2.26 for Thorney Island Trial 45. The conditions for the release are taken from [22]. The changes to the passive model for Version 2.27 have no effect on the results in the modelled range. This is found to be true also for the Thorney Island Trial 47 and for the previous comparisons [22] with Desert Tortoise and Burro Datasets.   We therefore conclude that the existing validation against dense gas datasets remains valid.

A1.6.2   Prairie Grass

To validate the passive model we compare with the Prairie Grass dataset included in the MDA [27]. The Prairie Grass experiments were conducted with SO_2 tracer released near ground level. The site (O'Neill, Nebraska) is flat and has a roughness length of only 6mm. Measurements of tracer were made on arcs and sampled (averaged) over the duration of each release (600s). The MDA suggests a receptor height of 1.5m for modelling purposes.

There are over 50 Prairie Grass Trials in the MDA, we have selected just 5 of these to cover different atmospheric conditions. PG9 and PG10 represent releases in unstable conditions, PG33 in neutral conditions, PG32 and PG36 releases in stable conditions.

DRIFT input conditions are taken from information given in the MDA. We have chosen to input the friction velocity and (inverse) Monin-Obukhov length for these releases.

DRIFT concentration predictions (specifying an averaging time of 600s) compared with experimental data are shown in Figure 18 to Figure 22.

Figure 18 shows predictions of DRIFT 2.27 and DRIFT 2.26 for trial PG9.

Based on these limited comparisons the adoption of the new passive formulation appears reasonable. The comparisons do show some tendency for the model to underpredict concentration for stable conditions and to overpredict concentration for unstable conditions. These may reflect the limitations of the DRIFT model for σ_v and the plume spread being assumed to be proportional to $\sigma_v / \overline{u}$.

A possible alternative to the passive lateral spread model is to use an empirical model for σ_y as given for example by Briggs [26]. This has been investigated and found to give slightly superior performance for the Prairie Grass cases looked at above.   For the moment we prefer the apparent generality of using $\sigma_v / \overline{u}$ with $\sigma_v = 2.0 u_*$, but note that this approach may not give optimal agreement with data.