

## **VALIDATION OF PHAST DISPERSION MODEL AS REQUIRED FOR USA LNG SITING APPLICATIONS**

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### **ABSTRACT**

PHMSA in consultation with FERC has issued guidance relating to approval in the USA of atmospheric dispersion models for LNG siting applications. This guidance includes a Model Evaluation Protocol (MEP), and an associated experimental database against which the model needs to be validated. Final approval was obtained in October 2011 for the Phast dispersion model UDM, and this paper summarises the submission of this model according to the above PHMSA guidance.

The UDM model is the main model in the hazard assessment software package Phast. It is a Unified Dispersion Model (UDM) for two-phase jet, heavy and passive dispersion including droplet rainout and pool spreading/evaporation. The UDM model can deal with a wide range of scenarios including both pressurised jet releases and unpressurised releases.

The paper first summarises the overall verification and validation of the UDM (both for LNG and other chemicals), which includes validation against experiments included in the REDIPHEN database (as produced as part of the EU project SMEDIS) and the MDA database (as produced by Hanna et al.). Subsequently the paper outlines UDM validation against experiments as required by the PHMSA for the LNG model evaluation protocol (MEP). This includes large-scale LNG field experiments involving dispersion from a liquid pool (Maplin Sands, Burro, Coyote) and large-scale Freon/Nitrogen field experiments involving dispersion from ground-level vapour area sources (Thorney Island). Overall very good agreement was obtained for the field experiments.

The results of the validation were submitted to PHMSA including required statistics for model accuracy (mean ratio observed to predicted, variance, etc.). The PHMSA submission also included detailed technical documentation for the UDM dispersion model (theory, verification and validation), and a report relating to conformance of the UDM against the model evaluation protocol (MEP). The authors believe that this type of model evaluation exercise is essential to ensure sufficient model accuracy and to gain community support.

### **1. INTRODUCTION**

The Pipeline and Hazardous Material Safety Administration (PHMSA) of the USA Department of Transportation (DOT) has issued standards (Regulation 49 CFR193) for safe design, siting, construction and operation of LNG facilities. These standards require that the operator or governmental authority control an 'exclusion zone' defined as the area that could be exposed to unsafe levels of thermal radiation or dispersion of flammable gas in case of a LNG release and ignition. In practice only one dispersion model was approved and available – DEGADIS, and this model has not been updated in a long time.

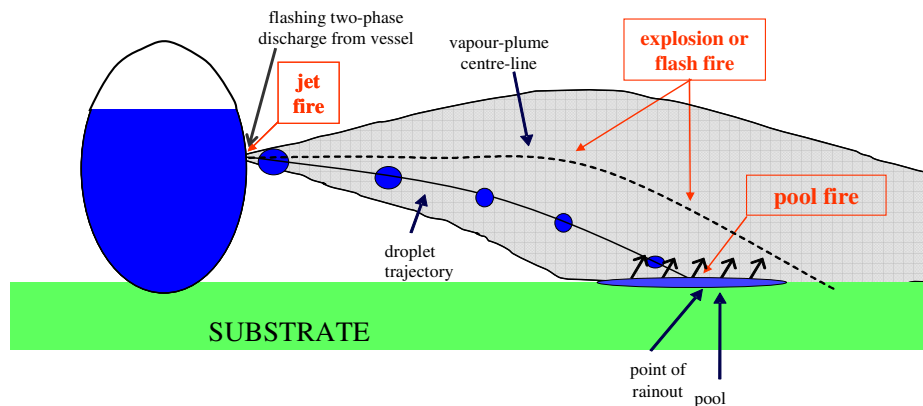
In conjunction with this standard, PHMSA in consultation with the Federal Energy Regulatory Commission (FERC) has issued guidance relating to approval of atmospheric dispersion models for LNG siting applications. This guidance is based on the Model Evaluation Protocol (MEP) developed by HSL (Coldrick et al., 2010), and an associated experimental database against which the model needs to be validated (Ivings et al., 2007). For further details see the FERC paper by Kohout (2012).

Final approval by the PHMSA was obtained in October 2011 for the dispersion model UDM contained in the hazard-assessment software package Phast developed by DNV Software. This paper summarises the submission of this model according to the above PHMSA guidance.

Section 2 provides an overview of UDM dispersion model. Section 3 summarises the overall verification and validation of the UDM (both for LNG and other chemicals). Section 4 subsequently outlines UDM validation against experiments as required by the PHMSA for the LNG model evaluation protocol (MEP). Section 5 summarises the overall submission of the Phast dispersion model UDM and its final approval by the PHMSA.

## 2. OVERVIEW OF PHAST DISPERSION MODEL UDM

The hazard-assessment package Phast (Witlox, 2010; Witlox and Oke, 2008) for consequence modelling of accidental releases of flammable or toxic chemicals to the atmosphere includes discharge, dispersion, toxic and flammable calculations. The flammable calculations include fireballs (instantaneous releases), jet fires (pressurised releases), pool fires (after rainout), and vapour cloud fires or explosion; see Figure 1 for the case of a continuous two-phase release of a flammable material with rainout. The UDM model is the main model in the hazard assessment software package Phast. It is a Unified Dispersion Model (UDM) for two-phase jet, heavy and passive dispersion including droplet rainout and pool spreading/evaporation.



**Figure 1. Continuous two-phase release of flammable material with rainout**

The UDM can model a wide range of scenarios. Distinction can be made between momentum (un-pressurised or pressurised releases), time-dependency (steady-state, finite-duration, instantaneous or time-varying dispersion), buoyancy (buoyant rising cloud, passive dispersion or heavy-gas-dispersion), thermodynamic behaviour (isothermal or cold or hot plume, vapour or liquid or solid or multiple-phase, reactions or no reactions), ground effects (soil or water, flat terrain with uniform surface roughness), and ambient conditions (stable, neutral or unstable conditions).

The UDM models the dispersion following a ground-level or elevated two-phase pressurised release. It effectively consists of the following linked modules (see Figure 1):

- jet dispersion
- droplet evaporation and rainout, touchdown
- pool spread and vaporisation
- heavy gas dispersion
- passive dispersion

A single form of concentration profile is used to cover all stages of a release. This allows for anything from a sharp-edged profile in the initial stages of a jet release through to the diffuse Gaussian profile that would be expected in the final passive stage of spreading.

The UDM includes the effects of droplet vaporisation using a non-equilibrium model. Rainout produces a pool which spreads and vaporises. Vapour is added back into the plume and allowance is made for this additional vapour flow to vary with time.

The UDM allows for vertical variation in ambient speed, temperature and pressure. Another feature of the UDM is possible plume lift-off, where a grounded cloud becomes buoyant and rises into the air. Rising clouds may be constrained to the mixing layer if it is reached.

For further details the reader is referred to the UDM overview paper by Witlox and Holt (1999), the Phast 6.7 theory manual for the UDM (Witlox and Harper, 2011a), its thermodynamic sub-module THRM (Witlox and Harper, 2011b) and pool evaporation sub-module PVAP (Witlox, 2011).

### **3. OVERALL PHAST (UDM) MODEL VERIFICATION AND VALIDATION**

The overall UDM validation includes validation against experiments stored in the MDA database by Hanna et al. (1993). It also includes validation against experiments included in the REDIPHEM database, which was carried out partly as part of the EU project SMEDIS (Daish et al., 1999). The SMEDIS project did produce a protocol for evaluating heavy gas dispersion models, which was the basis of the LNG model evaluation protocol proposed by Ivings et al. (2007). The SMEDIS project also included an independent peer review of the UDM model by Britter (2002). He states in this model evaluation report (MER) that the UDM model is amongst the most extensively documented and validated models.

The verification and validation for the individual UDM submodels can be summarised as follows [see Witlox and Harper (2011a,b) and Witlox (2011) for further details and a detailed list of references]:

- Jet and near-field passive dispersion. For an elevated horizontal continuous jet (of air), the UDM numerical results are shown to be identical to the results obtained by an analytical solution. For vertical jets very good agreement has been obtained against both the “Pratte and Baines” and “Briggs” empirical plume rise correlations.
- Heavy-gas dispersion. The UDM numerical results are shown to be in identical agreement against an analytical solution for a 2D isothermal ground-level plume. The UDM has been validated against the set of three 2D wind-tunnel experiments (McQuaid, 1976) and the isothermal HTAG wind tunnel experiments (Petersen and Ratcliff, 1988). Furthermore the UDM model was verified against the HGSYSTEM heavy-gas dispersion model HEGADAS.
- Far-field passive dispersion. For purely (far-field) passive continuous dispersion, the UDM numerical results are shown to be in close agreement with the vertical and crosswind dispersion coefficients and concentrations obtained from the commonly adopted analytical Gaussian passive dispersion formula. The same agreement has been obtained for the case of purely (far-field) passive instantaneous dispersion, while assuming along-wind spreading equal to cross-wind spreading in the analytical profile.
- Finite-duration releases. The UDM “Finite-duration-correction” module has been verified against the HGSYSTEM/SLAB steady-state results, and shown to lead to finite-duration corrections virtually identical to the latter programs. Furthermore excellent agreement was obtained using this module for

validation against the Kit Fox experiments (20-second releases of CO<sub>2</sub> during both neutral and stable conditions).

- Thermodynamics. The UDM dispersion model invokes the thermodynamics module while solving the dispersion equations in the downwind direction. This module describes the mixing of the released component with moist air, and may take into account water-vapour and heat transfer from the substrate to the cloud. The module calculates the phase distribution [component (vapour, liquid), water (vapour, liquid, ice)], vapour and liquid cloud temperature, and cloud density. Thus separate water (liquid or ice) and component (liquid) aerosols may form. The liquid component in the aerosol is considered to consist of spherical droplets and additional droplet equations may be solved to determine the droplet trajectories, droplet mass and droplet temperature. Rainout of the liquid component occurs if the droplet size is sufficiently large. The thermodynamics module also allows for more rigorous multi-component modelling (Witlox et al., 2006). The UDM homogeneous equilibrium model has been verified for both single-component and multi-component materials against the HEGADAS model. The UDM HF thermodynamics model (including effects of aqueous fog formation and polymerisation) was validated against the experiments by Schotte (1987).
- Release rate, initial droplet size and rainout validation. This relates to validation of both the Phast discharge model as well as the UDM dispersion model as carried out as part of a droplet modelling joint industry project (JIP). This includes validation of flow rate, initial droplet size and rainout against a wide range of experiments (Witlox and Harper, 2011c). This resulted in improvement of the droplet size correlation and rainout predictions in Phast.
- Pool spreading/evaporation. If the droplet reaches the ground, rainout occurs, i.e. removal of the liquid component from the cloud. This produces a liquid pool which spreads and vaporises (see Figure 1). Vapour is added back into the cloud and allowance is made for this additional vapour flow to vary with time. The UDM source term model PVAP calculates the spreading and vapour flow rate from the pool. Different models are adopted depending whether the spill is on land or water, and whether it is an instantaneous or a continuous release. The pool spreads until it reaches a bund or a minimum pool thickness. The pool may either boil or evaporate while simultaneously spreading. For spills on land, the model takes into account heat conduction from the ground, ambient convection from the air, radiation and vapour diffusion. These are usually the main mechanisms for boiling and evaporation. Solution and possible reaction of the liquid in water are also included for spills on water, these being important for some chemicals. These effects are modelled numerically, maintaining mass and heat balances for both boiling and evaporating pools. This allows the pool temperature to vary as heat is either absorbed by the liquid or lost during evaporation.

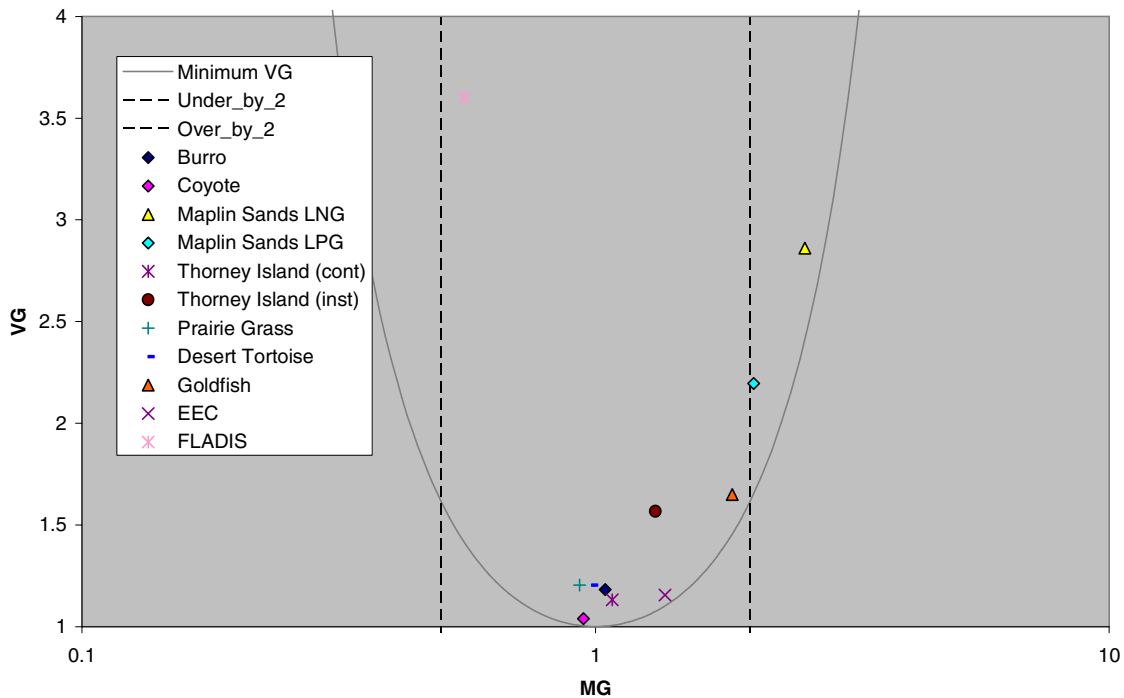
PVAP was verified by Webber (2003) against the SRD/HSE model GASP for a range of scenarios with the aim of testing the various sub-modules, and overall good agreement was obtained. The PVAP spreading logic was first validated against experimental data for spreading of non-volatile materials. Subsequently the PVAP evaporation logic was validated against experimental data in confined areas where spreading does not take place. Finally comparisons were made for simultaneously spreading and vaporising pools. The above validation was carried out for both spills on water and land, and a wide range of materials was included [LNG, propane, butane, pentane, hexane, cyclo-hexane, toluene, ammonia, nitrogen, water, Freon-11].

The validation of the overall UDM model was carried out against large-scale field experiments selected from the MDA and REDIPHEM databases, including the following:

- Prairie Grass (continuous passive dispersion of sulphur dioxide).
- Desert Tortoise and FLADIS (continuous elevated two-phase ammonia jet)
- EEC (continuous elevated two-phase propane jet)

- Goldfish (continuous elevated two-phase HF jet)
- Maplin Sands, Burro and Coyote (continuous evaporation of LNG from pool)
- Thorney Island (instantaneous un-pressurised ground-level release of Freon-12)
- Kit Fox (continuous and finite-duration heavy-gas dispersion of CO<sub>2</sub> from area source)
- BP Spadeadam (pressurised CO<sub>2</sub> release: cold steady-state releases and supercritical hot vapour releases)

Each of the above experimental sets was statistically evaluated to determine the accuracy and precision of the UDM predictions with the observed data. Formulas adopted by Hanna et al. (1993) were used to calculate the geometric mean bias MG (under or over-prediction of mean) and mean variance VG (scatter from observed data) for each validation run. A perfect result would have both MG and VG = 1. This was carried out for centre-line concentrations, cloud widths, and (for the SMEDIS experiments) also off centre-line concentrations. The overall performance of the UDM in predicting both peak centreline concentration and cloud widths was found to be good for the above experiments. A graphical presentation of the overall MG, VG validation results for arc-wise concentration (excluding CO<sub>2</sub> experiments) is shown in Figure 2. The figure also shows the factor of 2 band ( $0.5 < MG < 2$ ) expected from good quality similarity models. See the UDM validation manual for further details.



**Figure 2. Phast UDM Version 6.7 validation statistics (MG, VG) for maximum arc-wise concentration**

The overall UDM model was also verified by means of comparison against other models (HGSYSTEM, SLAB, TRACE, ALOHA, SCIPUFF) for three US chlorine accidents involving elevated two-phase chlorine jet releases, and the Phast predictions were found typically in the medium range of the predictions; see Hanna et al. (2007) for full details.

## 4. PHAST (UDM) VALIDATION AGAINST PHMSA EXPERIMENTS

This section outlines UDM validation against experiments as required by the PHMSA for the LNG model evaluation protocol (MEP). Full details are provided in the UDM validation document by Witlox and Harper (2011d) submitted to the PHMSA.

### 4.1 Selection of experiments

Table 1 lists the experiments against which the UDM model has been validated and also lists how each experiment has been modelled by the UDM:

- The large-scale LNG field experiments involve dispersion from a liquid pool (Maplin Sands, Burro, Coyote). These experiments have been modelled as low-momentum elevated horizontal releases (with immediate virtually 100% rainout).
- The large-scale Freon/Nitrogen field experiments involve dispersion from a ground-level vapour area sources (Thorney Island), and have been modelled as a low-momentum ground-level horizontal release.
- The CHRC, BA-Hamburg and BA-TNO scaled wind-tunnel experiments were modelled at full scale as a ground-level vapour pool source

Experiment	trial nr.	Type	Material	Modelled by UDM as
Maplin Sands	27,34,35	Field	LNG	Low momentum elevated horizontal release
Burro	3,7,8,9	Field	LNG	Low momentum elevated horizontal release
Coyote	3,5,6	Field	LNG	Low momentum elevated horizontal release
Thorney Island	45,47	Field	Freon&N <sub>2</sub>	Low momentum ground-level horizontal release
CHRC	A	Wind tunnel	CO <sub>2</sub>	Ground-level vapour pool source
BA-Hamburg	DA0120,DAT223	Wind tunnel	SF <sub>6</sub>	Ground-level vapour pool source
BA-TNO	TUV01,FLS	Wind tunnel	SF <sub>6</sub>	Ground-level vapour pool source

**Table 1. List of experiments for UDM validation**

### 4.2 UDM input and results

After rainout, the UDM model invokes the PVAP model for pool calculations and divides the time-varying pool evaporation rate into a number of segments (with constant evaporation rate during segment duration). The PHMSA includes both experimental maximum concentrations (one-second averaged), and (for Burro and Coyote) longer averaging-time measurements. For the short-averaging times, the pool segment is applied which produces the highest concentration. For the long averaging times, the pool segment most likely to be active in the given time-averaging window has been selected.

In line with the model evaluation protocol, the following UDM output data were produced:

- arcwise maximum concentration at measurement elevation and downwind distance
- distance to measured arcwise maximum concentration at measurement elevation

- arcwise cloud width at downwind distance where concentrations were measured
- point-wise concentrations at measurement location

The following UDM validation statistics were derived from the above results:

- MG (mean) and VG (variance) for above data [ratio observed to predicted; for each experiment and each group of experiments]
- MRB (mean relative bias) and MRSE (mean relative square error) [relative difference; for each group of experiments]
- FAC2 [fraction within factor of 2; for each groups of experiments]
- CSF (Concentration safety factor) [ratio predicted to observed; for each groups of experiments]
- LFL safety factors for LNG experiments (arcwise data only; LFL = 4.4%):
  - Concentration safety factor to LFL,  $CSF_{LFL}$  [ratio of predicted concentration (at observed distance to LFL) to LFL]
  - Distance safety factor to LFL,  $DSF_{LFL}$  [ratio of predicted to observed distance to LFL]

Table 2 lists the UDM input data for the example case of the Burro experiments (trials 3, 7, 8, 9). In this table the 'BU03' column, lists all the input data for BU03 experiment, while the subsequent columns indicate the input data of the trials BU07, BU08 and BU09 as far as they differ from BU03. Table 3 lists the observed and predicted results for these experiments. This includes UDM validation statistics (MG, VG for concentration and width; CSF).

Table 4 includes a list of MG, VG,  $CSF_{LFL}$ ,  $DSF_{LFL}$  values for the individual experiments in the LNG Model Validation Database. The same data are plotted for the field experiments in Figure 3. Figure 4 includes the combined MG and VG values for each group of experiments. The following is concluded from these tables and figures:

- Field experiments – short averaging times
  - Excellent results are obtained for the Burro and Coyote experiments
  - Maplin Sand under-predicts the concentrations.
- Field – long averaging times
  - Thorney Island gives excellent results
  - Burro give good results for both concentrations and cloud widths, though with slightly higher variance than for short averaging times
  - Concentrations are over-predicted for the Coyote experiments
- Wind-tunnel experiments
  - Concentrations are consistently under-predicted, while the cloud widths are slightly over-predicted. To maintain conservation of mass this appears to imply that either the cloud depth is over-predicted (too much heavy-gas entrainment at top of cloud) and/or the cloud speed is over-predicted
  - The above may be partly caused by inaccurate scaling. To further evaluate the cause an in-depth study of the un-scaled experiments would be desired first. It is recommended to do this as part of further work.

As previously indicated modelling Maplin Sands releases tends to produce large duration pool segments which will underestimate the actual peak evaporation rate. This will in turn lead to concentrations that are too low. The combination of significant time-varying effects and long averaging times is difficult to model with the Phast 'segment' approach, as it is difficult to choose a segment with an evaporation rate representative of the time-averaging window.

According to verbal communication with PHMSA/FERC, the above UDM under-prediction for the Maplin Sands experiments and the wind-tunnel experiments appears to be in line with other model predictions, and as such this may be caused by the quality of experimental data (Maplin Sand experiments) or inaccuracy of scaling (wind-tunnel experiments).

Description	Units	BU03	BU07	BU08	BU09	Notes
<b>RELEASE DATA</b>						
Duration		167	174	107	79	
Material		Methane				Assume LNG = pure methane
Release rate	kg/s	87.98	99.46	116.93	135.98	
Initial state [-1: saturated liquid at boiling point]		-1				Saturated liquid at its boiling point
Droplet size	m	0.01				Assume maximum permitted in Phast
Release height	m	1.5				
Release angle [0 = horizontal]	radians	0				
Release velocity (continuous only)	m/s	0.1				Assume minimum release velocity
<b>AMBIENT DATA</b>						
Pasquill stability class (5-C,7-D,8-E)		5	7	8	7	
Wind speed at reference height	m/s	5.58	8.75	1.94	5.94	
Reference height for wind speed	m	3				
Temperature at reference height	K	307.75	306.96	306.02	308.52	
Pressure at reference height	N/m2	94840.2	94029.6	94130.925	94029.6	
Reference height for temperature and pressure	m	1				
Atmospheric humidity (fraction)	-	0.052	0.074	0.045	0.144	
<b>SUBSTRATE DATA</b>						
Surface roughness length	m	0.0002				
Dispersing surface type (1-land,2-water)		1				
<b>POOL DATA</b>						
Surface [5:deep water (no ice), 8:shallow water]		8				
Temperature of pool surface	K	307.75	306.96	306.02	308.52	
Bund diameter (= 0: no bund)	m	0				
<b>AVERAGING TIME</b>						
Averaging time	s	100	140	80	50	

**Table 2. Burro experiments - UDM input data (long averaging time)**

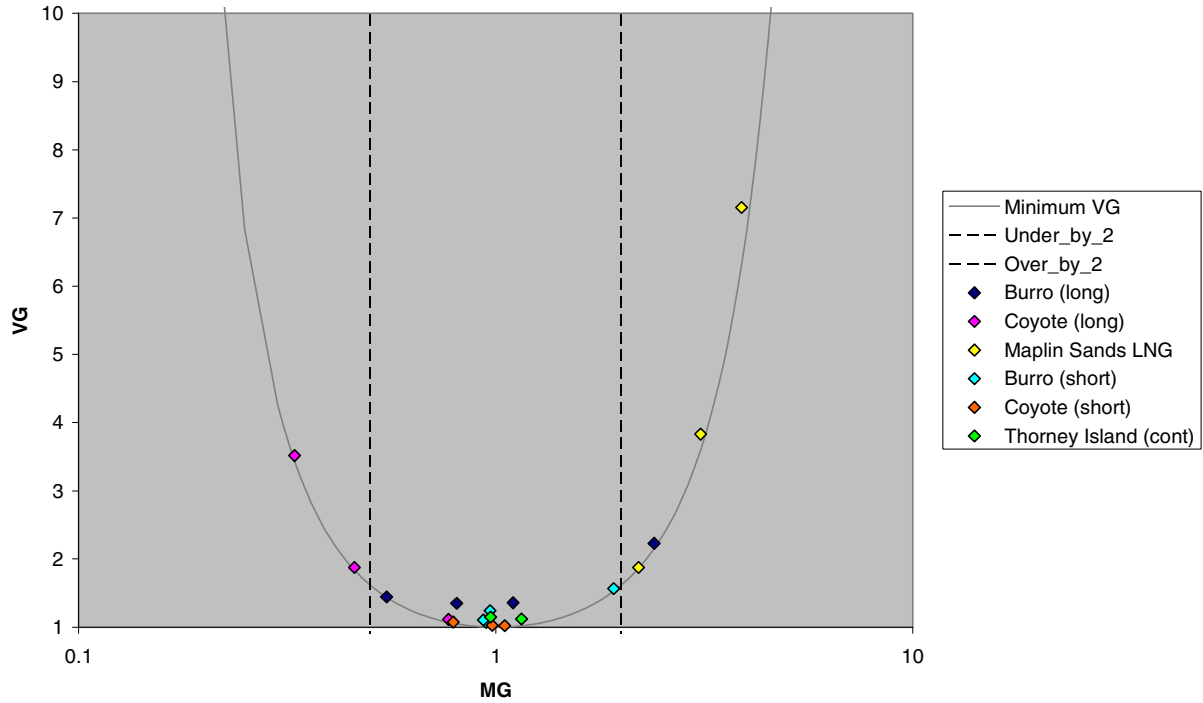
Experiment ID	Downwind distance m	Height of interest m	Concentration observed mol%	Concentration predicted mol%	Width observed m	Width predicted m	Concentration Mean MG	Variance VG	Width Mean MG	Variance VG	CSF (cp/co)	
<b>Burro (long)</b>	BU07	57	1	14.19	17.01	-1.00	14.00	0.81	1.35	1.14	1.02	1.20
		140	1	4.40	10.30	20.50	18.03					2.34
		400	1	2.29	1.56	-1.00	26.17					0.68
	BU08	57	1	30.67	16.03	28.80	85.08	2.40	2.23	0.56	1.80	0.52
		140	1	16.36	5.52	-1.00	87.81					0.34
		400	1	3.50	1.71	87.04	93.37					0.49
		800	1	2.08	0.73	-1.00	101.02					0.35
	BU09	140	1	6.52	12.47	30.90	24.21	1.10	1.36	1.41	1.13	1.91
		400	1	2.79	2.07	49.20	32.46					0.74
	800	1	1.16	0.61	61.60	42.20					0.53	
BU03	57	1	7.89	15.56	20.86	18.76	0.55	1.45	1.11	1.01	1.97	
	140	1	6.11	10.35	-1.00	24.34					1.69	
<b>Burro (short)</b>	BU07	57	1	17.90	20.10	-1.00	26.04	0.97	1.24	-1.00	-1.00	1.12
		140	1	7.13	12.41	-1.00	33.23					1.74
		400	1	3.86	2.17	-1.00	43.91					0.56
	BU08	57	1	55.87	22.62	-1.00	178.27	1.91	1.56	-1.00	-1.00	0.40
		140	1	16.49	10.07	-1.00	194.10					0.61
		400	1	4.27	2.51	-1.00	200.50					0.59
		800	1	2.12	1.09	-1.00	210.01					0.52
	BU09	140	1	10.56	17.17	-1.00	55.76	0.93	1.11	-1.00	-1.00	1.63
		400	1	3.96	3.83	-1.00	72.20					0.97
		800	1	1.40	1.09	-1.00	85.56					0.78
	BU03	57	1	22.40	18.25	-1.00	35.28	0.95	1.07	-1.00	-1.00	0.81
		140	1	8.98	12.24	-1.00	45.25					1.36

**Table 3. Burro experiments – UDM validation against arcwise concentration & width**

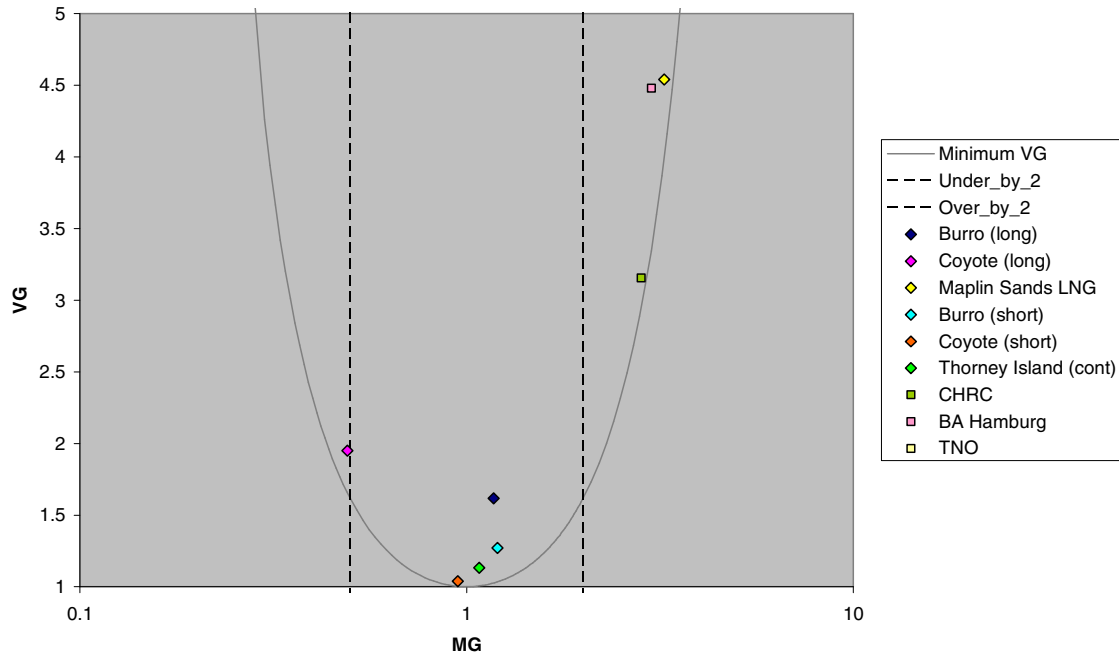


Type experiment	Experiment	Trial nr.	Arcwise Concentration		Width		Pointwise Concentration		CSF <sub>LFL</sub>	DSF <sub>LFL</sub>
			MG	VG	MG	VG	MG	VG		
			MG	VG	MG	VG	MG	VG		
Field - Short Averaging time	Maplin Sands	27	3.89	7.15	-	-	-	-	0.23	0.36
		34	2.20	1.88	-	-	-	-	0.47	0.58
		35	3.10	3.83	-	-	-	-	0.41	0.55
	Burro	3	0.95	1.07	-	-	1.09	1.08	0.79	0.91
		7	0.97	1.24	-	-	0.82	4.01	0.78	0.88
		8	1.92	1.57	-	-	0.95	1.35	0.6	0.62
		9	0.93	1.11	-	-	1.02	1.17	1.1	1.04
	Coyote	3	0.79	1.08	-	-	1.36	1.37	1.4	1.15
		5	1.05	1.02	-	-	1.47	2.05	1.13	1.03
		6	0.98	1.03	-	-	0.62	1.75	1.02	1.01
Field - Long Averaging time	Burro	3	0.55	1.45	1.11	1.01	0.31	6.23	0.22	0.51
		7	0.81	1.35	1.14	1.02	0.47	9.82	2.34	1.69
		8	2.40	2.23	0.56	1.80	1.06	1.31	0.49	0.51
		9	1.10	1.36	1.41	1.13	1.14	1.81	1.54	1.23
	Coyote	3	0.46	1.87	1.46	1.15	0.64	1.63	2.05	1.47
		5	0.33	3.52	-	-	0.40	3.79	3.88	3.44
		6	0.77	1.11	1.07	1.14	0.38	6.49	1.43	1.19
	Thorney Island	45	1.15	1.12	-	-	-	-	-	-
		47	0.97	1.15	-	-	-	-	-	-
	Windtunnel - Pool Source	CHRC	A	2.83	3.16	0.60	1.33	1.94	2.69	-
Hamburg		DA0120	3.89	6.78	-	-	-	-	-	-
		DAT223	1.51	1.48	-	-	1.92	1.79	-	-
TNO		TUV01	-	-	-	-	2.74	3.72	-	-
		FLS	3.49	5.23	0.84	1.07	3.34	6.34	-	-

**Table 4. List of MG, VG, CSF<sub>LFL</sub> and DSF<sub>LFL</sub> values for experiments**



**Figure 3. Plot of MG and VG values (arcwise concentrations) for individual field experiments**

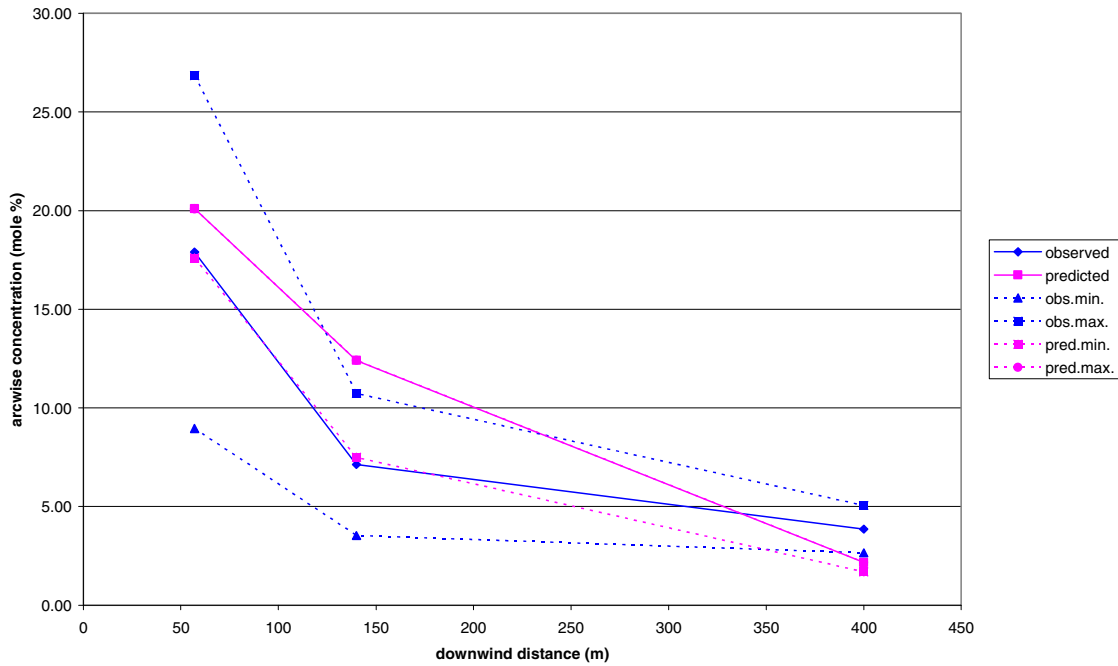


**Figure 4. Plot of MG and VG values (arcwise concentrations) for each group of experiments**

### 4.3 Sensitivity analysis

This submission also included a sensitivity analysis. This includes sensitivity to the experimental uncertainty of the input parameters (wind speed, stability class, surface roughness, ambient pressure, humidity, LNG mixture composition) and a sensitivity analysis to deviations to the measured maximum arc-wise concentrations.

This sensitivity analysis is illustrated in Figure 5 for the case of Burro 7 (short averaging time). Here the observed value and absolute deviations from the mean (downwards and upwards) were provided by FERC/PHMSA (2011). Figure 5 illustrates the inaccuracy in measuring the concentrations (blue curves/markers), versus the spread in the model predictions (pink curves/markers) resulting from the range of input variations as given by FERC/PHMSA. For this specific case, the maximum prediction concentration corresponded to the base-case, while the minimum prediction concentrations corresponded to a higher value of surface roughness (10mm versus base-case value of 0.2mm) and mixture composition (exact composition versus base-case assumption of pure methane).



**Figure 5. Burro 7 (short) - Measured versus observed concentrations**

## 5. PHAST (UDM) SUBMISSION AND PHMSA APPROVAL

The results of the validation presented in the previous section were submitted to PHMSA including all required UDM validation statistics for model accuracy. The PHMSA submission also included detailed technical documentation for the UDM dispersion model (theory, verification and validation), and a report relating to conformance of the UDM against the model evaluation protocol (MEP).

Final approval was obtained in October 2011 for the Phast dispersion model UDM by the PHMSA. The approval was obtained for both versions 6.6 and 6.7 of the Phast software. Both versions produce virtually identical results for dispersion from ground-level LNG pools (using new UDM ‘Version 2’ solver), but the new version 6.7 includes more advanced rainout modelling for elevated two-phase releases (Witlox and Harper, 2012).

The approval was obtained for scenarios involving dispersion from circular shaped LNG pools, dispersion from LNG pools in impoundments with low aspect ratios, and dispersion from releases in any direction (including releases from flashing, venting and pressure relief). Although the Phast dispersion model UDM has been validated against line sources (as describe in Section 3; validation against McQuaid experiments), this feature has currently not yet been made available in Phast. Furthermore Phast currently presumes dispersion over terrain with a uniform surface roughness. Thus the PHMSA decision acknowledged that the current Phast may not be appropriate for dispersion from high aspect-ratio pools (e.g. trenches), across highly varying terrain, or around large obstacles. Furthermore PHMSA recommended that the UDM is used with a safety factor of 2 (i.e use 0.5 LFL) to account for turbulent fluctuations and model uncertainties. This is in line with the Phast default settings for flammable materials.

While DNV is pleased to note approval of Phast, we have commented to PHMSA that real releases involve complex source term aspects (flashing, drop size distributions, rain-out, pool formation and re-evaporation) not included in the PHMSA list of validation experiments. Thus other CFD models, which may appear superficially to be superior to Phast (UDM) in the dispersion over varying terrain aspect, may in fact be deficient in their less sophisticated source-term modelling and overall predicted results may not be superior. Issues related to a CFD model may also include numerical accuracy/convergence, appropriate selection of grid, turbulence model (to account for e.g. heavy-gas-dispersion effects) and boundary conditions (e.g. wall laws etc.). Thus many different CFD results could be obtained depending on the chosen input. Furthermore the extensive CPU time does often not allow repetitive runs in order to obtain more confidence in the CFD results.

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## REFERENCES

Britter, R., 2002, Model Evaluation Report on UDM Version 6.0, Ref. No. SMEDIS/00/9/E, Version 1.0, 21 January 2002, Prepared by Cambridge Environmental Research Consultants Ltd, Cambridge, UK

Coldrick, S., Lea, C.J. and Ivings, M.J., 2010, "Validation database for evaluating vapour dispersion models for Safety Analysis of LNG facilities", Guide to the LNG model validation database, Health and Safety Laboratory, Revision May 2010

Daish, N.C, Britter, R.E., Linden, P.F., Jagger, S.F. and Carissimo, B., 1999, "SMEDIS: Scientific Model Evaluation Techniques Applied to Dense Gas Dispersion models in complex situations"., *Int. Conf. and workshop on modelling the consequences of accidental releases of hazardous materials*, San Francisco, California, CCPS, New York, 345-372

FERC/PHMSA, "Sensitivity bounds and experimental uncertainty", Memo provided by FERC/PHMSA in email from Charles Helm dated 3 March 2011

Hanna, S.R., Chang, J.C. and Strimaitis, D.G., 1993, "Hazardous gas model evaluation with field observations", *Atm. Env.*, 27a: 2265-2285

Hanna, S., Dharmavaram, S., Zhang, J., Sykes, I., Witlox, H. W. M., Khajehnajafi, S. and Koslan, K., 2007, "Comparison of six widely-used dense gas dispersion models for three actual chlorine railcar accidents", *Proceedings of 29th NATO/SPS International Technical Meeting on Air Pollution Modelling and its Application*, 24 - 28 September 2007, Aveiro, Portugal

Ivings, M.J., Jagger, S.F., Lea, C.J. and Webber, D.M., 2007, "Evaluating vapor dispersion models for safety analysis of LNG facilities", Contract by HSL for Fire Protection Research Foundation, Quincy, Massachusetts

Kohout, A., 2012, "Evaluation of dispersion models for LNG siting applications", Session LNG Plant Safety and Protection, 12<sup>th</sup> *Topical Conference on Gas Utilization*, AIChE Spring Meeting, April 2012

McQuaid, J., 1976, "Some experiments on the structure of stably stratified shear flows", Technical Paper P21, Safety in Mines Research Establishment, Sheffield, UK

Nedelka, D., Moorhouse, J., and Tucker, R. F., 1990, "The Montoir 35m diameter LNG pool fire experiments", *Proc. 9<sup>th</sup> Intl. Cong and Exposition on LNG*, LNG9, Nice, 17-20 October 1989, Published by Institute of Gas technology, Chicago, 2-III-3: 1-23

Petersen, R.L. and Ratcliff, M.A., 1988, "Effect of homogeneous and heterogeneous surface roughness on HTAG dispersion", CPP Incorporated, Colorado. Contract for API, Draft Report CPP-87-0417

Schotte, W., 1987, "Fog formation of hydrogen fluoride in air", *Ind. Eng. Chem. Res.*, 26: 300-306; see also Schotte, W., "Thermodynamic model for HF formation", 31 August 1988, Letter from Schotte to Soczek, E.I. Du Pont de Nemours & Company, Du Pont Experimental Station, Engineering Department, Wilmington, Delaware 19898

Webber, D., 2003, "PVAP Theory Document", distributed as part of Phast 6.7 software, DNV Software, London

Witlox, H.W.M. 2010, "Overview of consequence modelling in the hazard assessment package Phast", Paper 7.2, 6<sup>th</sup> AMS conference on applications of air pollution meteorology, Atlanta, USA, 17-21 January 2010

Witlox, H.W.M., 2011, "PVAP Theory Document", UDM Version 6.7, distributed as part of Phast 6.7 software, DNV Software, London

Witlox, H.W.M. and Harper, M. 2011a, "UDM Theory Document," UDM Version 6.7, distributed as part of Phast 6.7 software, DNV Software, London

Witlox, H.W.M. and Harper, M. 2011b, "UDM Thermodynamics Theory Document," UDM Version 6.7, distributed as part of Phast 6.7 software, DNV Software, London

Witlox, H.W.M. and Harper, M., 2011c, "Two-phase jet releases, droplet dispersion and rainout, I. Overview and model validation", 14<sup>th</sup> Annual Symposium, Mary Kay O'Connor Process Safety Centre, Texas A&M University, College Station, Texas, 25-27 October 2011, pp. 642-655 also accepted for publication in *Journal Loss Prevention*

Witlox, H.W.M. and Harper, M. 2011d, "Validation of Phast dispersion model UDM against experiments in LNG Model Validation Database" (submission to PHMSA/FERC), DNV Software, London, April 2011

Witlox, H.W.M., Harper, M., Topalis, P. and Wilkinson, S., 2006, "Modelling the consequence of hazardous multi-component two-phase releases to the atmosphere", *Hazards XIX Conference*, Manchester, 250-265

Witlox, H.W.M. and Holt, A., 1999, "A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation", *International Conference and Workshop on Modelling the Consequences of Accidental Releases of Hazardous Materials*, CCPS, San Francisco, California, September 28 – October 1, 315-344

Witlox, H.W.M. and Oke, A., 2008, "Verification and validation of consequence models for accidental releases of hazardous chemicals to the atmosphere", *Hazards XX Conference*, Manchester, 14-17 April 2008