CHEMICAL ENGINEERING TRANSACTIONS
VOL. 31, 2013
Guest Editors: Eddy De Rademaeker, Bruno Fabiano, Simberto Senni Buratti

ISBN 978-88-95608-22-8; ISSN 1974-9791
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet
DOI: 10.3303/CET1331009

Validation of PHAST Dispersion Model as Required for USA LNG Siting Applications

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PHMSA in consultation with FERC 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. Approval was obtained for the PHAST dispersion model UDM, and this paper summarises the submission of this model according to the above PHMSA guidance.

1. Introduction

The Pipeline and Hazardous Materials 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 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. For further details the reader is referred to the more detailed paper by Witlox et al. (2012).
Section 2 provides an overview of the UDM dispersion model including model verification and validation. Section 3 subsequently outlines UDM validation against experiments as required by the PHMSA for the LNG MEP. Section 4 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) 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 is the core 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 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,

Please cite this article as: Witlox H., Harper M. and Pitblado R., 2013, Validation of phast dispersion model as required for usa lng siting applications, Chemical Engineering Transactions, 31, 49-54 DOI: 10.3303/CET1331009

reactions or no reactions), ground effects (soil or water, flat terrain with uniform surface roughness), and ambient conditions (stable, neutral or unstable conditions).

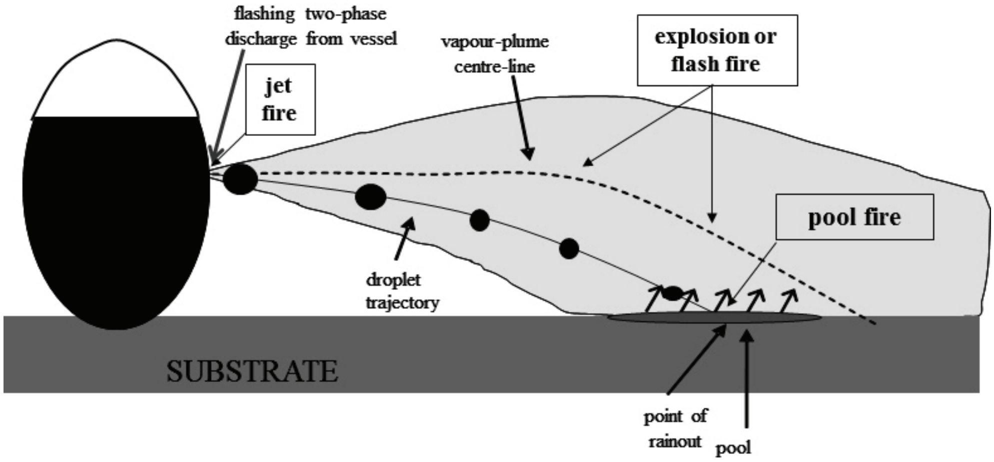

Figure 1: Continuous two-phase release of flammable material with rainout

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 and passive dispersion

Witlox et al. (2012) include further details of the verification and validation for the individual UDM sub-models. This includes the dispersion regimes of near-field jet dispersion, heavy-gas dispersion and passive dispersion. In addition it includes the thermodynamics module for mixing air with the released pollutant, including droplet break up and evaporation, rainout and pool spreading/evaporation. It finally includes verification and validation for short-duration releases.

In addition the UDM has been validated against large-scale experiments recorded in the MDA (Hanna et al. 1993) and REDIPHEM databases. This validation was carried out partly as part of the EU project SMEDIS (Daish et al., 1999). The SMEDIS project produced 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.

Large-scale experimental datasets considered include:

- 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 short-duration heavy-gas dispersion of CO_2 from area source)
- BP and Shell Spadeadam (pressurised CO_2 release: cold steady-state liquid releases, time-varying cold liquid releases, and time-varying 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. Overall predictions were within a factor of 2 ($0.5 < MG < 2$) and with a small variance ($1 < VG < 2$), expected from good quality similarity models. See Witlox et al. (2012) for further details.

The UDM 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.

3. Phast (UDM) validation against PHMSA specified 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 (2011) submitted to the PHMSA (Docket No. 2011-0075).

3.1 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 and 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.

Table 1: List of experiments for UDM validation

Experiment	trial number	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_2	Low momentum ground-level horizontal release
CHRC	A	Wind	CO2	Ground-level vapour pool source
BA-Hamburg	DA0120,DAT	Wind	SF_6	Ground-level vapour pool source
BA-TNO	TUV01,FLS	Wind	SF_6	Ground-level vapour pool source

3.2 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 each segment). 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. With the exception of these case data, all model inputs were the defaults in Phast 6.7. Table 3 lists the observed and predicted results for these experiments. This includes UDM validation statistics (MG, VG for concentration and width). 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 2. 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 gives 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 is recommended as part of further work.

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

Description	BU03	BU07	BU08	BU09	Notes
RELEASE DATA					
Duration (s)	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]	-1				Saturated liquid at boiling point
Droplet size (m)	0.01				Assume maximum allowed value
Release height (m)	1.5				
Release angle [radians; 0 = horizontal]	0				
Release velocity (m/s)	0.1				Assume min. release velocity
AMBIENT DATA					
Pasquill stability class	C	D	E	D	
Wind speed (m/s) at reference height	5.58	8.75	1.94	5.94	
Reference height (m) for wind speed	3				
Temperature (K) at reference height	307.75	306.96	306.02	308.52	
Pressure (N/m^2) at reference height	94840	94030	94131	94030	
Reference height (m) for temperature and pressure	1				
Atmospheric humidity (%)	5.2	7.4	4.5	14.4	
SUBSTRATE DATA					
Surface roughness length (m)	0.0002				
Dispersing surface type	land				
POOL DATA					
Surface [8:shallow water (with possibly ice)]	8				
Temperature (K) of pool surface	307.75	306.96	306.02	308.52	
Bund diameter (= 0: no bund)	0				
Averaging time (s)	100	140	80	50	

Table 3: Burro experiments – UDM validation against arcwise concentration & width (long averaging time)

Test	Downwind distance	Height of interest	Concentration observed	predicted	Width obs.	pred.	Concentration Mean	Variance	Width Mean	Variance
	m	m	mol%	mol%	m	m	MG	VG	MG	VG
BU07	57	1	14.19	17.01		14.00	0.81	1.35	1.14	1.02
	140	1	4.40	10.30	20.50	18.03				
	400	1	2.29	1.56		26.17				
BU08	57	1	30.67	16.03	28.80	85.08	2.40	2.23	0.56	1.80
	140	1	16.36	5.52		87.81				
	400	1	3.50	1.71	87.04	93.37				
	800	1	2.08	0.73		101.0				
BU09	140	1	6.52	12.47	30.90	24.21	1.10	1.36	1.41	1.13
	400	1	2.79	2.07	49.20	32.46				
	800	1	1.16	0.61	61.60	42.20				
BU03	57	1	7.89	15.56	20.86	18.76	0.55	1.45	1.11	1.01
	140	1	6.11	10.35		24.34				

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).

Table 4: List of MG, VG, CSF_{LFL} and DSF_{LFL} values for experiments

Type experiment	Experiment	Trial number	Arcwise concentration		Width		Pointwise concentration		CSF_{LFL}	DSF_{LFL}
			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	1.91	1.56	-	-	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	-	-	-	-	0.00	0.00		
		FLS	3.49	5.23	0.84	1.07	3.34	6.34		

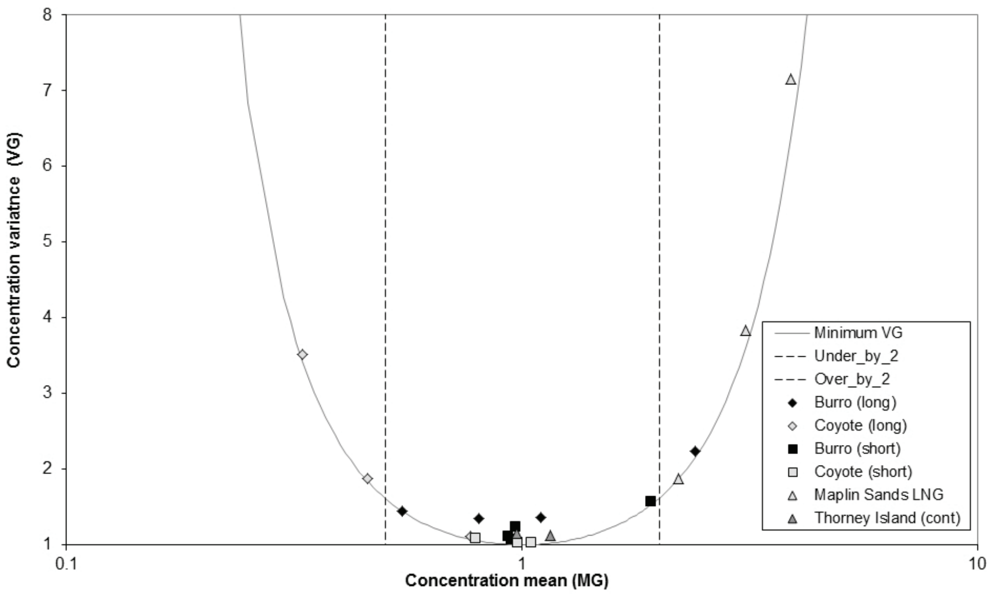

Figure 2: Plot of MG and VG values (arcwise concentrations) for individual field experiments

4. 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. This submission also included a sensitivity analysis 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. Also detailed technical documentation was provided (theory, verification and validation), and details on UDM conformance 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, 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. PHMSA also 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.

5. Conclusions

The Phast dispersion model UDM has been validated against the field experiments in the PHMSA database. Overall good agreement has been obtained for concentration predictions against the field experiments, and over-prediction against the scaled wind tunnel experiments may have been caused by incorrect scaling.

The results of the above validation along with detailed technical documentation and a sensitivity analysis has been submitted to PHSMA, and following this the UDM model has been approved for USA LNG siting applications.

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, Buxton, UK,

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, USA, 345-372

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, Buxton, UK

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

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

Witlox, H.W.M. and Harper, M. 2011, 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., and Pitblado, R., "Validation of Phast dispersion model as required for USA LNG Siting Applications", LNG plant safety symposium, 12th topical conference on gas utilisation AICHE Spring Meeting, April 2012