Journal of Hazardous Materials, 6 (1982) 107—128 107
Elsevier Scientific Publishing Company, Amsterdam — Printed in The Netherlands

HEAVY GAS DISPERSION MODELS

D.R. BLACKMORE,
Shell Research Ltd., Thornton Research Centre, P.O. Box 1, Chester CH1 3SH (Gt. Britain)
M.N. HERMAN and J.L. WOODWARD
Exxon Research and Engineering Co., P.O. Box 101, Florham Park, New Jersey 07932 (U.S.A.)
(Received November 2, 1981; accepted November 24, 1981)

Summary

This paper reviews fifteen current mathematical models for the dispersion of accidental releases of heavy gases until they dilute with air to non-flammable or non-toxic concentrations. The models are broadly classified into K-theory models (5 in number) and slab models (10 in number). In addition, 4 jet release models are given that can describe elevated releases of heavy gases.

For each model, a description is given of the mechanistic features claimed, the applicability to differing types and geometries of release, the ease of availability to users, and the degree to which calculated results have been compared with field data. To facilitate comparison, these characteristics are listed in a common tabular form for each model.

1. Introduction

Mathematical modelling of the dispersion of the vapours resulting from accidental releases of volatile liquids and heavy gases has been helpful in establishing safe designs and operating procedures for the transport and storage of flammable and toxic materials. The experimental data which became available in the early 1970's made it evident that a new class of models was required to describe the phenomena observed. Heavy vapours usually form low, flat clouds which spread because of their own density even in the absence of wind. It was recognized that attempting to describe such systems by adapting Gaussian models suitable for neutrally or positively buoyant clouds was inherently inadequate [1]. Consequently, many models have been proposed*, though often after only a limited comparison of the predictions with experimental data.

*These models are being surveyed by a working group under the auspices of the UK's CIA, and an abbreviation of this survey is presented in this paper.

One objective of heavy vapour dispersion models has been the prediction of the effects of a very large spill of liquefied natural gas (LNG) onto water, such as may occur after an accidental collision involving an LNG carrier. The sudden release of the contents of a cargo tank containing 25,000 m^3 LNG has been defined by the U.S. Coast Guard as a "credible spill". In his 1978 review, Havens [2] showed that a number of models produced widely varying estimates for the distance to which a flammable cloud would extend under a wind of 5 miles per hour. Since that time, the range of the estimates represented by the model predictions in Havens's report has narrowed as modellers have refined their simulations. Some of the models used in Havens's report are now considered obsolete and superseded by revised versions. A recent comparison of model predictions with experimental data by Woodward et al. [3] showed quite close agreement of the predictions of four of the more recent models. This comparison involved fairly small spills, but there is reason to expect model predictions for large spills to also converge as the uncertainty in heavy vapour cloud modelling decreases.

Present models designed to deal with heavy gases are usually placed into one of two categories: K-theory (eddy diffusivity) models and slab (also known as top-hat or box) models, although some models do not fit neatly into either category. K-theory models numerically integrate suitably simplified equations of mass, momentum, and energy conservation, in either two- or three-dimensional form. In principle, K-theory models can incorporate terrain effects and complex geometries, and describe wake effects around structures. Mass transfer is assumed to be proportional to concentration gradients and to occur by eddy diffusion. The application of this type of model to density-stratified layers requires the extension of diffusivities and viscosities obtained either quasi-theoretically or experimentally from physically related phenomena (such as boundary layer meteorology).

Slab (or top-hat) models assume that mass transfer occurs by entrainment across the density interface of a cloud with an assumed shape (frequently cylindrical, or at least with vertical sides and a horizontal top) and that internal mixing is fast enough for the concentration within the cloud to be uniform. Air entrainment velocities are assumed to depend on turbulence levels, density differences, and cloud speed. Entrainment velocities are determined from laboratory experiments or by comparing model predictions to data from field experiments. This approach, like K-theory, is an idealization, since real vapour clouds are rarely cylindrical or perfectly flat-topped, and the motion of entrainment velocity may oversimplify complex phenomena. The test of any model is how well it extrapolates to situations beyond those for which the model parameters were adjusted.

As a heavy gas cloud dilutes, it will reach a point where it is no longer heavy (i.e., its density becomes close to that of the surrounding air). At this stage, it is important (if the cloud is still flammable or toxic) that the correct mathematical description be given of the subsequent neutrally buoyant dispersion. Some models require a specific (and sudden) transition from a negatively buoyant to a neutrally buoyant dispersion mechanism; others account for this transition naturally and continuously.

Sources of heavy gases, like models, are also usually classified according to two ideal types: continuous sources (steady-state liquid pools, for instance, or small ruptures in a pipe or vessel) and instantaneous sources (severely ruptured vessels, for instance, or rapidly emptying pressurized tanks). From the first type of source, an unvarying plume of heavy gas will be formed if the source lasts long enough, and continuous or steady-state plume models suffice. From the second type of source, a "puff" of heavy gas will be formed which will be advected downwind, and will grow and dilute with distance downwind. In this case, an instantaneous heavy gas model applies. A real heavy vapour source, however, such as a liquid pool which is both spreading and vaporizing, will be neither continuous nor instantaneous, but will vary in time. Of those few models which can treat this type of source, most incorporate three-dimensional K-theory. Also, an approach to adapting steady-state models to time-varying sources has been described by Colenbrander [4], which works well for all cases except those with very low wind speeds.

All heavy gas dispersion models suffer from the fact that good data on the dispersion of heavy gas clouds are scarce. Thus, many models are not validated adequately. Comparisons can be and have been made only with the various (normally small-scale) data that exist. The least desirable situation, which is happily becoming rarer, is the development of a so-called "model" which is little more than a means of numerically reproducing a particular set of field data. Confidence in the general application (e.g. extrapolation to larger spills) of such "models" is clearly limited.

2. Available models

Overall characteristics of models currently in use are listed in Table 1 and described in more detail in Tables 4a—c. Comparisons with experimental data are shown in Table 2 and the experimental data are summarized in Table 3. Models regarded as obsolete are listed in Table 5. We include in the tables only those models which have been published in the open literature. We are aware of a few models that have not yet reached the stage of publication, and others that are more recent or developing versions of published models, but both these categories are excluded from this survey.

Table 1 indicates the types of sources each model was designed to treat. Blow-down calculations and calculations of liquid pool spread and vaporization are usually done with separate models, but it is possible to couple such source models directly to heavy vapour dispersion models.

A number of comparisons of model predictions with experimental findings have been made, and Table 2 shows our evaluation of all of which we are aware. Unfortunately, not all such comparisons have been published, so independent verification of the conclusions indicated may not be possible. We can only urge authors to publish all such comparisons in the future.

TABLE 1

Overview of model capabilities

Model name or author	"Instantaneous" gas cloud (Burst or Puff)	Steady continuous source; plume concentrations independent of time				Variable continuous source; plume concentrations dependent on time				
Models for ground level releases		Elevated source	Point on the ground	Line	Confined area source	Elevated source	Point on the ground	Line	Confined area source	Spreading area source
K-Theory models										
ZEPHYR [5]	S	P	S	S	S	P	S	S	S	S
TRANSLOC [6]	S	P	S	S	S	P	S	S	S	S
SIGMET-N [7]	S	P	S	S	S	P	S	S	S	S
MARIAH [8]	S	P	S	S	S	P	S	S	S	S
DISCO [9]	S	P	S	S	S	P	R	R	R	R
Slab models										
HEGADAS II [4]	S		S	S^*	S		S	S^*	S	S
Cox and Carpenter [10]	S		S	S^*	S^+			R	R	P
Eidsvik [11–13]	S		S	S^*	S^+					S
Fay [14]	S									
Flothmann & Nikodem [15]	S			P^*	P^+					
DENZ [16]	S		S	S^*	S^+					
Germeles and Drake [17]	S		S	S^*	S^+					
Picknett [18,19]	S									
van Buijtenen [20]	S		P	P	P		S	S	S	S
van Ulden [21]	S									
Models for jet releases										
Astleford et al. [22]		S	S							
Bloom [23]		S	S							
Cox et al. [24]		S	S							
Ooms et al. [25]		S	S							

Code

S = Model is suitable for the type of source indicated.

R = Model requires repetitive runs to handle the source indicated.

P = Model applies in principle.

* = Line source perpendicular to wind direction.

\+ = Treated as a vertical rectangular source.

TABLE 2

Comparisons of models with experimental data [a]

Model name or author	Data on composition and cloud dimensions			Data on cloud dimensions only		Other unpublished comparisons [b]	Other published comparisons [c]
	Esso/API (1972)	AGA (1974)	HSE/ Porton Down (1978)	van Ulden (1974)	Shell 'Gadila' (1974)		
Models for ground level releases							
K-Theory models							
ZEPHYR [5]	CA [3,5]		CA [3,5]	CA [5]		RC [29]	
TRANSLOC [6]							
SIGMET [26,27]	C [30]	CA [30]	CA [30]				
SIGMET-N [7]							
MARIAH [8]	CA [3,8]		CA [3,8]	RC [3,8]			
DISCO [9]						RC [29,31]	
Slab models							
HEGADAS II [4]	CA [4,3]	CA [4,3]	CA [3]			CA [32]	
Cox and Carpenter [10]			[10]*	C [10]	CA [10]		
Eidsvik [11—13]	C [3]		CA [11,13]*				
Fay [14]	C [14]		RC [14]	CA [14]		C [14,33]	
Flothmann & Nikodem [15]				[15]*			
DENZ [16]							C [31,34,35,36,37]
Germeles and Drake [17]			C [3]			RC [31,38]	
Picknett [18,19]			[18]*				
van Buijtenen [20]	[20]*			[20]*			
van Ulden [21]				[21]*			
Jet release models for elevated sources							
Astleford et al. [22,28]						CA [22,28] [d]	CA [25,39,40]
Bloom [23]							
Cox et al. [24]						CA [25] [d]	CA [25,39,40]
Ooms et al. [25]						CA [25] [d]	CA [25,39,40]

Code
CA = Comparison made and close agreement between model results and data was found.
* = Comparison made and model was calibrated to data.
RC = Comparison made and rough consistency between model results and data was found.
C = *Comparison made.*

[a] For brief descriptions of experiment, see Table 3.
[b] Comparison claimed by authors but unverified and unpublished. References to data cited.
[c] Both original data and comparison with data in references cited.
[d] Unpublished wind tunnel or plume observations.

TABLE 3

Heavy gas generation and dispersion experiments

Tests and references	Number of spills and sizes	Duration or rate	Surface	Comments
LNG				
Esso—API, 1972 [41]	17 at 0.73 to 10 m^3	~20 m^3/min	Water	Vaporization and dispersion study
Gaz de France, 1972 [42]	18 at up to 3 m^3	Instantaneous	Dry bund	Dispersion study
Battelle—Columbus, 1974 [43,44]	42 at 0.4 to 51 m^3	~20 sec	Soils (Two 24 m bunds)	
Shell 'Gadila', 1974 [45]	6 at 27 to 200 m^3	Up to 20 m^3/min	Sea water	Liquid jettisoning test; only photographic evidence
China Lake, DOE, 1978 [46]	4 at ~4.5 m^3	4 m^3/min	Water	Pool spread, dispersion; instrument evaluation exercise
Freon 12				
DGA (Min. of Social Affairs) Netherlands, 1974 [1,47]	1 at 1 tonne	Vaporized in 5 sec	Land	Dispersion study
HSE/Porton, 1978 [18]	39 at 100 kg	Instantaneous	Land	Dispersion study
Ammonia (actual accidents)				
Potchefstroom S. Africa, 1973 [34]	30 tonnes	Instantaneous	Land	Tank accident
Houston, Texas, 1976 [35]	19 tonnes	Instantaneous	Land	Road tanker accident

TABLE 4a

K-Theory models (Models are listed alphabetically according to the author's surname)

Model name	ZEPHYR	TRANSLOC (heavy gas version)	SIGMET-N	MARIAH	DISCO
General description	Numerical, 3-Dimensional transient heavy gas model	A K-Model modified for describing heavy gas clouds	Numerical, 3-Dimensional transient heavy gas model	Numerical, 3-Dimensional transient heavy gas model	Numerical, 2-Dimensional steady-state heavy gas model; uses stream function
Author	W.G. England and W. McBride	G. Schnatz and D. Flothmann	F.Y. Su and P.C. Patnak	J.R. Taft	L.H. Tauscher
Affiliation	Energy Resources Co., Inc., La Jolla, CA, USA	Battelle, Frankfurt F.R.G.	Science Applications, Inc. El Segundo, CA, USA	Deygon-Ra, Inc., La Jolla, CA, USA	Energy Resources Co. Inc., La Jolla, CA, USA
Reference	[5]	[6]	[7]	[8]	[9]
Is a written computer listing available?	Yes	Yes	Yes	Yes	Yes
1. Conditions treated					
(A) Sources and types of spill (see Table 1)	All	All	All	All	Requires multiple runs for time-varying source
(B) Types of release					
— jet momentum	Possibly (with fine grid)	No	Possibly (with fine grid)	Possibly (with fine grid)	No
— buoyant plume	Yes	No	Yes	Yes	Yes
— aerosol	No	Yes	No	No	No
(C) Dispersing regimes					
— open	Yes	Yes	Yes	Yes	Yes
— obstructed (wakes)	Yes	No	Yes	Yes	No
— topography (variable terrain)	Yes	No	Yes	Yes	No
— deposition from cloud	No	Yes	No	No	No

TABLE 4a (cont.)

	ZEPHYR	TRANSLOC (heavy gas version)	SIGMET-N	MARIAH	DISCO
(D) Meteorology					
— atmospheric stability	Yes	Yes	Yes	Yes	Yes
— very low wind speed (<1 m/sec)	Yes	No	Yes	Yes	No
— humidity and heat of condensation	Yes	No	Yes	Yes	Yes
2. Mechanistic features					
(A) Air-entrainment treatment	3-Dimensional K-theory; Particle-in-cell Lagrangian diffusion	2-Dimensional K-theory modified from nuclear fallout model with variable terrain	3-Dimensional K-theory	3-Dimensional K-theory, uses implicit form of equations	2-Dimensional K-theory; steady-state
(B) Transition from gravity spreading/entrainment to nonbuoyant passive dispersion	Not needed, use rezoning	Not needed	Not needed, use rezoning	Not needed, automatic rezoning	Not needed
(C) Heat transfer from surface to gas cloud	Yes	No	Yes	Yes	Yes
(D) Other significant features		Momentum balances not solved	Allows water vapour entrainment		

TABLE 4b

Slab models (Models are listed alphabetically according to the author's surname)

Model name	HEGADAS II	Cox and Carpenter	Eidsvik	Fay	Flothmann and Nikodem
General description	Transient behaviour of heavy gas clouds from area sources	Heavy gas cloud behaviour	Heavy gas cloud behaviour	Heavy gas cloud behaviour	Heavy gas cloud behaviour
Author	G.W. Colenbrander	R.A. Cox and R.J. Carpenter	K. Eidsvik	J.A. Fay	D. Flothmann and H.J. Nikodem
Affiliation	Shell Research	Cremer & Warner/ British Gas	Norwegian Inst. for Air Research	Mass. Inst. of Tech.	Batelle, Frankfurt, FRG
Reference	[4]	[10]	[11–13]	[14]	[15]
Is a written computer listing available?	No	No	No	No	Yes
1. *Conditions treated*					
(A) Sources and types of spill (see Table 1)	Instantaneous, constant and time-varying (horizontal rectangular) sources	Instantaneous (cylindrical) and constant (vertical rectangular) sources	Instantaneous (cylindrical, with time-varying gas input) and constant (vertical rect-angular) sources	Instantaneous (cylindrical source)	Instantaneous (cylindrical) and constant (vertical rectangular) sources
(B) Types of release					
— jet momentum	No	No	No	No	No
— buoyant plume	No	No	No	No	No
— aerosol	No	No	No	No	Yes, for thermo-dynamic equilibrium behaviour
(C) Dispersing regime					
— open	Yes	Yes	Yes	Yes	Yes
— obstructed (wakes)	No	Yes (by an approximate method)	No	No	No

TABLE 4b (cont.

	HEGADAS II	Cox and Carpenter	Eidsvik	Fay	Flothmann and Nikodem
— topography (variable terrain)	No	No	No	No	No
— deposition from cloud	No	No	No	No	No
(D) Meteorology					
— atmospheric stability	Yes	Yes	Yes	Yes	Yes
— very low wind speed (<1 m/sec)	No	Yes	Yes	Yes	No
— humidity and heat of condensation	Yes	Yes	Yes	Yes	Yes
2. Mechanistic features					
(A) Air-entrainment treatment	Dispersion in vertical and horizontal directions dependent on atmospheric turbulence; vertical dispersion is also a function of Richardson number: similarity concentration profiles assumed	Entrainment velocity for top-surface mixing is a function of atmospheric turbulence and Richardson number: entrainment velocity for edge mixing is dependent on gravity spreading velocity: well-mixed cloud assumed	Entrainment velocity for top-surface mixing is a function of atmospheric and convective turbulence and Richardson number: entrainment velocity for edge mixing is dependent on gravity spreading velocity: well-mixed cloud assumed	Entrainment velocity for top-surface mixing is a function of atmospheric turbulence and independent of Richardson number: edge mixing not important in the later stages: well-mixed cloud assumed	Entrainment velocity for top-surface mixing is a function of atmospheric turbulence and Richardson number: entrainment velocity for edge mixing is dependent on gravity spreading velocity: Gaussian concentration profiles assumed
(B) Transition from gravity spreading/entrainment to nonbuoyant dispersion	Continuous and smooth	When lateral turbulence velocity > lateral gravity spread velocity	Continuous and smooth	No transition	Continuous and smooth
(C) Heat transfer from surface to gas cloud	No	Yes	Yes	No	Yes
(D) Other significant features	The "observer concept" accounts for the time-varying sources	Thermodynamics of 2-phase mixtures included		Not a model that describes the growth of the cloud: it only gives predictions when highly diluted	

TABLE 4b (cont.)

Model name	DENZ	Germeles and Drake	Picknett	van Buijtenen	van Ulden
General description	Heavy gas cloud behaviour	Heavy gas cloud behaviour	Heavy gas cloud behaviour	Transient behaviour of heavy gas clouds from area sources	Heavy gas cloud spreading behaviour
Author	L.S. Fryer and G.D. Kaiser	A.E. Germeles and E.M. Drake	R.G. Picknett	C.J.P. van Buijtenen	A.P. van Ulden
Affiliation	U.K. Atomic Energy Authority	Cabot Corp. and A.D. Little	Chemical Defence Est., Porton (HSE contract)	TNO, Netherlands	KNMI (Royal Netherlands Met. Inst.)
Reference	[16]	[17]	[18,19]	[20]	[1,21]
Is a written computer listing available?	No	Yes (via Cabot Corp.)	No		No
1. *Conditions treated*					
(A) Sources and types of spill (see Table 1)	Instantaneous (cylindrical) source	Instantaneous (cylindrical) and constant (vertical rectangular) sources	Instantaneous (cylindrical) source	Instantaneous, constant and time-varying sources	Instantaneous (cylindrical) source
(B) Types of release					
— jet momentum	No	No	No	No	No
— buoyant plume	No	No	No	No	No
— aerosol	No	No	No	No	No
(C) Dispersing regimes					
— open	Yes	Yes	Yes	Yes	Yes
— obstructed (wakes)	No	No	No	No	No
— topography (variable terrain)	No	No	No	No	No
— deposition from cloud	No	No	No	No	No
(D) Meteorology					
— atmospheric stability	Yes	Yes, in Gaussian portion	Yes	Yes	Yes
— very low wind speed (<1 m/sec)		Yes	Yes	Yes	Yes
— humidity and heat of condensation		Yes	Yes	Yes	No

TABLE 4b (cont.)

	DENZ	Germeles and Drake	Picknett	van Buijtenen	van Ulden
2. Mechanistic features					
(A) Air-entrainment treatment	Entrainment velocity for top-surface mixing is a function of atmospheric turbulence and Richardson number: no edge mixing: well-mixed cloud assumed	Entrainment velocity for top-surface mixing is a function of gravity spreading velocity and Richardson number: no edge mixing: well-mixed cloud assumed	Entrainment velocity for top-surface mixing is a function of atmospheric turbulence and Richardson number: entrainment velocity for edge mixing is dependent on gravity spreading velocity: well-mixed cloud assumed	Take-up rates from an assumed stationary gas-pool above the liquid pool: Gaussian plume treatment with empirically modified vertical dispersion coefficients equivalent to Pasquill F behaviour	Only cloud radius treated in published description; extension expected in future publication to air entrainment with edge and top-surface mixing as function of Richardson number
(B) Transition from gravity spreading/entrainment to nonbuoyant dispersion	When density difference between cloud and air becomes less than specified value	When cloud edge speed equals wind speed	When an eddy can reach the ground ($3\sigma_w$ = height of cloud or Richardson number = 1)	Not needed: gas entrained from the gas-pool is considered to be the source	When Richardson number equals 0.5
(C) Heat transfer from surface to gas cloud	Yes	Yes	No	No	No
(D) Other significant features	Alternative transition criterion (B): if the radial increase due to gravitational slumping does not exceed that due to turbulence alone, and the top entrainment velocity is greater than the longitudinal turbulence velocity	Gaussian sub-model allows virtual-point and line sources	Relates to Porton data only	The "observer concept" accounts for the time-varying sources	

TABLE 4c

Jet-release models for elevated sources (Models are listed alphabetically according to the author's surname)

Model name	Astleford et al.	Bloom	Cox et al.	Ooms et al.
General description	Descending plume and ground level heavy gas metal	Heavy gas plume path where gas is reactive	Heavy gas plume and cloud behaviour — plume converting to ground level cloud	Plume path of heavy gases
Author	W.J. Astleford, T.B. Morrow, R.J. Magott and R.L. Bass	S.G. Bloom	R.A. Cox, M.A. Pyman, P.A. Sheppard and J.P.S. Cooper	G. Ooms, A.P. Mahieu and F. Zelis
Affiliation	Southwest Research Inst., San Antonio, TX, USA	Battelle, Columbus, USA	Cremer and Warner	Shell Research
Reference	[22,28]	[23]	[24]	[25]
Is a witten computer listing available?	Yes	Yes	Yes	Yes
1. Conditions treated				
(A) Sources and types of spill (see Table 1)	Continuous jet release from point source; makes use of Ooms [25] heavy gas plume path model and te Riele [48] heavy gas cloud model	Continuous elevated release from point or finite area source	Continuous elevated point source; makes use of Ooms [25] heavy gas plume path model and Cox and Carpenter [10] heavy gas cloud model	Continuous jet release from point source
(B) Types of release				
— jet momentum	Yes	Yes	Yes	Yes
— buoyant plume	Yes	Yes	Yes	Yes
— aerosol	No	No	No	No
(C) Dispersing regimes				
— open	Yes	Yes	Yes	Yes
— obstructed (wakes)	No	No	No	No

TABLE 4c (cont.)

	Astleford et al.	Bloom	Cox et al.	Ooms et al.
— topography (variable terrain)	No	No	No	No
— deposition from cloud	No	Allows for reactive gases	No	No
(D) Meteorology				
— atmospheric stability	Yes	Yes	Yes	Yes
— very low wind speed (<1 m/sec)	Yes	Yes	Yes	Yes
— humidity and heat of condensation	No	Yes	No (but ground level model part does)	No
2. Mechanistic features				
(A) Air-entrainment treatment	Heavy gas behaviour is followed once the plume centreline hits the ground: entrainment rates of air into the plume depend on jet action, buoyancy and ambient turbulence	Entrainment rates of air into the plume depend on jet action, buoyancy close to the source and ambient turbulence further away	Heavy gas behaviour is followed once the plume centreline hits the ground; entrainment rates of air into the plume depend on jet action, buoyancy and ambient turbulence	Wind drag force across the plume is allowed for; entrainment rates of air into the plume depend on jet action, buoyancy and ambient turbulence
(B) Transition from gravity spreading/entrainment to passive dispersion	Continuous and smooth	Not needed	As for Cox and Carpenter [10]	Not needed
(C) Heat transfer from surface to gas cloud	No	Not in referenced version of model	As for Cox and Carpenter [10]	Not relevant
(D) Other significant features		Not designed to describe events after the plume reaches the ground. Energy equation includes phase changes, chemical reactions, and gain (or loss) of materal, including rainout of particles		Not designed to describe events after the plume reaches the ground

TABLE 5

Some obsolete heavy gas models

Author and reference	Model name	Company affiliation	Model replaced by
(a) Models for pool evaporation and cloud dispersion			
P.H.M. te Riele [48]	—	Shell Research	HEGADAS II [4]
D.S. Burgess et al. [49,50]	—	US Bureau of Mines	[see 2]
J.A. Fay and D.H. Lewis [51]	-	MIT	Fay [14]
G.F. Feldbauer et al. [41]	—	US API	[see 2]
—	CHRIS	USCG	[see 2]
—	FPC	US Federal Power Commission	[see 2]
H.J. Nikodem et al. [52,53]	—	Battelle, Frankfurt	Flothmann & Nikodem [15]
(b) Models for cloud dispersion only			
R.A. Cox and D.R. Roe [54]	—	Cremer & Warner (with British Gas)	Cox & Carpenter [10]
K.J. Eidsvik [11]	1st version	Norwegian Inst. of Air Research	2nd version [12,13]
G.D. Kaiser and B.C. Walker [55]	DENZ	SRD, Risley (UKAEA)	Fryer and Kaiser [16]

Tables 4a—c list model availability and characteristics. Note that the term "diffusion" is sometimes used to distinguish air/vapour mixing on the cloud edges from air entrainment into the bulk of the cloud. This artificial distinction is used primarily with slab models which may assume very sharp concentration gradients on the cloud boundaries (where no "diffusion" is allowed) while still diluting the overall cloud concentrations by air entrainment into the bulk of the cloud.

Some of the slab models listed in Table 4b are "advanced" in the sense that they each contain at least one feature beyond simple slab or top-hat theory*. For example, the HEGADAS II [4] model initially uses near-Gaussian composition profiles in the vertical dimension and on the edges of the cloud. Also, this model overcomes the limitations of being a steady-state model by means of repeated model runs using "observers" released to float over the cloud and report what they "see." This "observer" method is quite general and could, in principle, be extended to other models. Table 4b also lists the Eidsvik model [11—13], which incorporates asymptotically correct functions of physical variables in place of constant entrainment velocities. Both HEGADAS II and the Eidsvik model provide a smooth, natural transition to neutral buoyancy Gaussian models, as does the Flothmann and Nikodem model [15].

Models developed for atomic energy applications will usually be able to

*A good summary of the basic theory is given by Havens [56].

describe fallout and, to a limited extent, reactions (such as the hydrolysis of UF_6). One such model, TRANSLOC [6], has recently been improved so that it considers aerosol formation and evaporation. This capability is not generally available elsewhere, but since aerosol phenomena can also play an important part in the thermal balance in the cloud, future models may need to incorporate it.

Some models specifically address the release of heavy gases from an elevated stack or vent. Except for Bloom's model, all those listed in Tables 1 and 4c are based on Ooms's plume path computer model [25], which can describe both momentum jets and plumes with positive or negative buoyancy. Under certain circumstances the plume that is produced from an elevated source will follow a descending path, and then disperse as a continuous heavy gas cloud when the gases reach the ground. In a similar manner, jet release of heavy gas from a ground level vent can form a heavy gas cloud rapidly diluted by momentum effects, followed by less rapid dilution effects at ground level. Some modellers [22,24] have treated these situations by marrying a plume path model that can describe descending plumes to a heavy gas ground-level model. For details of the way transition between the two parts of each model is achieved, see the original papers.

3. Experimental data available to support the models

A selection of heavy gas dispersion experiments is listed in Table 3 and a fuller account is to be found in a following paper in this issue [57]. Comparisons with specific models are shown in Table 2. A recent and more detailed comparison of five particular models with certain spills from these experimental programmes is given in another paper in this issue [3].

Prior to 1980, experimental spills were all in the range of 1—11 m^3 of liquid. More recently, spills of up to 20 m^3 of liquid methane (LNG) and refrigerated propane have been conducted by Shell Research Ltd. (the Maplin Sands tests), but the results have not yet been fully reported*. Spills of 40 m^3 of LNG have been conducted by the U.S. Department of Energy (at China Lake, California), and the results are also expected soon*. These releases are within the range of expected accidental releases for spills on land. For spills over the ocean, the maximum release of LNG is usually considered to be 25,000 m^3, the size of a single storage tank on an LNG transport ship. The dispersion behaviour of gas clouds generated from spills of this order of magnitude might be affected by physical processes which are not accurately described from the relatively small scale experimental work done so far. Thus, there is still felt to be a need for data from well instrumented release of large quantities of gas in low winds. Spills of around 350 m^3 of LNG are being discussed in the United States [59]. Good experi-

*Preliminary accounts of both the Maplin (1980) and the China Lake (1980) experiments are to be found in later papers in this issue [57,58].

mental data from spills of this size would reduce the necessary scale-up to the large postulated spills by an order of magnitude and therefore improve confidence in model predictions for very large spills.

4. Assumptions of the models

Particular models often make specific assumptions, as indicated in Tables 4a–c. However, some assumptions are generally made by most models. These include:

(1) The dispersing cloud moves over flat terrain or water.
(2) The ground (or water) has constant roughness.
(3) The ground (or water) has constant thermal properties.
(4) There are no obstructions to the wind or moving cloud.
(5) The contaminant gas undergoes no chemical or physical reaction during dispersion (though one or two models designed for atomic energy applications are exceptions).
(6) Local concentration fluctuations are not predicted.

K-theory models can relax the assumptions of flat terrain and of no obstructions, within the limitations of computer capacity.

Slab or top-hat models apply additional assumptions:

(1) The cloud has a flat top.
(2) The concentration of contaminant is uniform across the cloud or, using a more general assumption, similarity profiles of velocity or concentration are imposed on the gas cloud.
(3) The cloud slumping velocity is described by the "gravity intrusion" models*.

5. Data and input parameters required by the models

Data required to describe the release rate, pool spread, and vaporization include:

(1) The physical properties of the spilled material: molecular weight, density, temperature, boiling point, latent heat of vaporization, etc.
(2) The physical properties of the substrate: heat capacity, thermal conductivity, etc.
(3) The nature of the spill: type (instantaneous, continuous, or time-varying), size (volume or volume rate), source (point, line, pool, elevated), type of release (momentum jet, buoyant plume, flash vaporization, etc,), initial state of release (dilution with air, liquid aerosol content).

*A recent paper discusses gravity flow in the inertial and viscous regimes [60].

Additional data required by cloud dispersion models are:

(1) The nature of the dispersing regime: roughness of surface, surface temperature, the degree of water pick-up in the boiling process (which may be important for LNG spills on water).

(2) Atmospheric conditions: wind speed, wind velocity profile, stability category (Pasquill or other localized definition), inversion layer height (if this affects the cloud), air temperature and humidity, barometric pressure.

Model parameters include the following:

(1) Diffusion coefficients (for 'K' models) in the y and z directions (and also x direction for instantaneous spills).

(2) The vapour production rate and source radius (if not already calculated).

(3) A gravity spreading constant.

(4) Entrainment coefficients (for slab models).

(5) The shape and dimensions of the cloud edge and top surface.

(6) Forced and free convective heat transfer coefficients.

6. Use of model computations

The principal parameter of interest in any particular application is the distance to the point where the cloud is no longer ignitable or toxic. For flammable vapours, this is commonly defined as the distance to the LFL (lower flammability limit), which is, for example, 5 vol.% for methane and 2 vol.% for propane. Of particular interest is the predicted extent of a flammable cloud at any time following a spill. At present, the dependencies of the predictions of different models on, for example, size of spill or windspeed are not in agreement. Thus, some models show a steady increase of dispersion distance with windspeed while others show windspeed to decrease dispersion distance, to have no effect on it, or to cause it to go through a maximum as the wind speed changes. The models also show that spill characteristics, weather stability, and humidity can all significantly affect dispersion behaviour.

Downwind dispersion distance is not the only parameter that can be calculated, or the only parameter of interest. The width and height of the flammable or toxic cloud can be relevant as well as the concentration as a function of time at a fixed location. Also, the extent of the visible cloud is a matter of significant practical interest. (There is, however, no general relationship between the visible edge and the gas concentration: for cold clouds, determination of the visible edge requires the effects of ambient humidity and heat transfer to be carefully modelled.)

Calculations are frequently made to the LFL/2 concentration distance, rather than to the LFL distance, on the grounds that small volumes ("pockets") of vapour can have concentrations considerably greater than the time-averaged concentration. Making the calculation in this way, of course, greatly increases the maximum downwind distance calculated (usually by a factor of about 1.5, but this depends on the model and on the vapour release conditions). There is little quantitative evidence to support this procedure, least of all for heavy-gas dispersion phenomena. However, in circumstances where it is used, it is reasonable to assume it over-estimates the distance at which the cloud is no longer ignitable. This is clearly an area where research is required in the future.

7. Acknowledgements

This paper stems from a review carried out by the UK Chemical Industry Association's Gas Dispersion Working Group, as part of CIA's Hazard Analysis study chaired by T.A. Kletz. Thanks are due to our fellow members of the Working Group, S.D. Green (BP Chemicals), N.C. Harris (ICI Mond), P.R.H. Jones (Esso Chemicals) chairman, and G.T. Sheppard (BNF) for the many discussions and much guidance in what was essentially a collaborative effort. Thanks are also due to J.S. Puttock (Shell Research Ltd., Thornton) and G.W. Colenbrander (Shell Research BV, Amsterdam) for their comments and advice during the writing of this paper.

References

1 A.P. van Ulden, On the spreading of a heavy gas released near the ground, Proc. 1st Int. Symp. on Loss Prevention and Safety Promotion in the Process Industries, Delft, Netherlands, 1974, pp. 221—226.
2 J.A. Havens, An assessment of predictability of LNG vapor dispersion from catastrophic spills into water, Paper C2, Proc. 5th Int. Symp. on the Transport of Dangerous Goods by Sea and Inland Waterways, Hamburg, F.R.G., 1978. A fuller report was issued by the USCG, Cargo & Hazardous Materials Division, Washington, DC.
3 J.L. Woodward, J.A. Havens, W.C. McBride, and J.R. Taft, A comparison with experimental data of several models for dispersion of heavy vapor clouds, J. Haz. Mat., 6 (1982) 161—180.
4 G.W. Colenbrander, A mathematical model for the transient behaviour of dense vapour clouds, 3rd Int. Symp. on Loss Prevention and Safety Promotion in the Process Industries, Basel, Switzerland, 1980.
5 W.C. McBride, A denser than air vapor dispersion validation study using the ZEPHYR and DISCO Models. A report by Energy Resources Company to Exxon Research & Engineering Company, 1981.
6 G. Schnatz and D. Flothmann, A 'K' model and its modification for the dispersion of heavy gases, in: S. Hartwig (Ed.), Heavy Gas and Risk Assessment, D. Reidel Publishing Co., Dordrecht, Holland, 1980, p. 125.
7 SIGMET-N Model Description and Users' Guide, SAI-236-81-232-LJ, Vols. 1 and 2 Science Applications, Inc., El Segundo, California, July 1981.
8 J.R. Taft, Simulations of experimental spills using MARIAH model, A report by Deygon—Ra, Inc., to Exxon Research & Engineering Company, 1981.
9 LNG terminal risk assessment study for Oxnard, California, Science Applications, Inc., prepared for Western LNG. Associates, 1975.

10 R.A. Cox and R.J. Carpenter, Further development of a dense vapour cloud dispersion model for hazard analysis, in S. Hartwig (Ed.), Heavy Gas and Risk Assessment, D. Reidel Publishing Co., Dordrecht, Holland, 1980, p. 55.
11 K.J. Eidsvik, Dispersion of heavy gas clouds in the atmosphere, Report No. 32/78, Norwegian Institute for Air Research, Lillestrøm, Norway, 1978.
12 K.J. Eidsvik, A model for heavy gas dispersion in the atmosphere, Atm. Env., 14 (1980) 769.
13 K.J. Eidsvik, Heavy gas dispersion model with liquefied release. Atm. Env., 15 (1981) 1163.
14 J.A. Fay, Gravitational spread and dilution of heavy vapor clouds, 2nd Int. Symp. on Stratified Flows, Vol. 1, Tapir, Trondheim, Norway, 1980, p. 471.
15 D. Flothmann and H.J. Nikodem, A heavy gas dispersion model with continuous transition from gravity spreading to tracer diffusion, in: S. Hartwig (Ed.), Heavy Gas and Risk Assessment, D. Reidel Publishing Co., Dordrecht, Holland, 1980, p. 89.
16 L.S. Fryer and G.D. Kaiser, DENZ — A computer program for the calculation of the dispersion of heavy toxic or explosive gases in the atmosphere, 1979, SRD R152, UKAEA.
17 A.E. Germeles and E.M. Drake, Gravity spreading and atmospheric dispersion of LNG vapor clouds, Fourth Int. Symp. on Transport of Hazardous Cargoes by Sea and Inland Waterways, Jacksonville, Florida, 1975.
18 R.G. Picknett, Field experiments on the behaviour of dense clouds, Chemical Defence Establishment, Porton Down, Salisbury, Wilts., Gt. Britain, Report No. IL 1154/78, 1978.
19 R.G. Picknett, Diffusion of dense gas puffs released in the atmosphere at ground level, Atm. Env., 15 (1981) 509.
20 C.J.P. van Buijtenen, Calculation of the amount of gas in the explosive region of a vapour cloud released in the atmosphere, J. Haz. Mat., 3 (1980) 201.
21 A.P. van Ulden, The Unsteady Gravity Spread of a Dense Cloud in a Calm Environment, NATO/CCMS Conference, Nov. 1979.
22 W.J. Astleford, T.B. Morrow, R.J. Magott, and R.L. Bass, USCG Report No. CG-D-41-79 (NTIS A072912), 1979.
23 S.G. Bloom, A mathematical model for reactive, negatively buoyant atmospheric plumes, in S. Hartwig (Ed.), Heavy Gas and Risk Assessment, D. Reidel Publishing Co., Dordrecht, Holland, 1980, p. 103.
24 R.A. Cox, M.A. Pyman, P.A. Sheppard, and J.P.S. Cooper, Models for evaluating the probabilities and consequences of possible outcomes following releases of toxic or flammable gases, in: S. Hartwig (Ed.), Heavy Gas and Risk Assessment, D. Reidel Publishing Co., Dordrecht, Holland, 1980, p. 185.
25 G. Ooms, A.P. Mahieu, and F. Zelis, Plume Path of Heavy Gases, 1st Int. Symp. on Loss Prevention and Safety Promotion in the Process Industries, The Hague, 1974.
26 W.G. England, L.H. Teuscher, L.E. Hauser, and B. Freeman, Atmospheric dispersion of liquefied natural gas vapor clouds using SIGMET, a three-dimensional, time-dependent hydrodynamic computer model, Heat Transfer and Fluid Mechanics Institute, Washington State University, 1978.
27 J.A. Havens, A description and assessment of the SIGMET LNG vapor dispersion model, U.S. Coast Guard Report CT-M-3-79, 1979.
28 T.B. Morrow, W.J. Astleford, R.J. Magott and R.L. Bass, The dispersion of chemical vapors emitted from marine chemical carrier, 3rd International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Basel, Switzerland, 1980.
29 D.E. Neff, R.N. Meroney, and J.E. Cermak, Wind tunnel study of the negatively buoyant plume due to an LNG spill, Colorado State University Report CER76-77 DEN-RNM-JEC 22, 1978.
30 J.R. Taft and W.C. McBride, Validation studies on dense gases using the SIGMET simulation model, Report EAI-RA-79-005, 1979, available from Lee Bell, Western LNG Terminal Associates, 700 S. Flower St., Los Angeles, Cal., 90017.

31 Railroad Accident Report; Louisville and Nashville Railroad Company freight train derailment and puncture of anhydrous ammonia tank car at Pensacola, Florida, November 9, 1977, US National Transportation Safety Board Report Number NTSB-RAR-78-24, 1978.
32 M.L. Barad [Ed.], Project prairie grass, a field program in diffusion, Geophysical Research Paper No. 59, Vols. I and II, AFCRC-TR-58-235, Air Force Cambridge Research Centre, Bedford, Mass., 1958.
33 D.J. Hall, Further experiments on a model of an escape of heavy gas, report LR(312)AP, Warren Springs Laboratory, Stevenage, Herts., Gt. Britain, 1974.
34 H. Lansdale, Ammonia tank failure in South Africa, Ammonia Plant Safety, 17 (1975) 126.
35 G. McMullen, A review of the 11th May ammonia truck accident, City of Houston Health Dept. Report, 1976.
36 G.D. Kaiser, Examples of the successful application of a simple model for the atmospheric dispersion of dense cold vapours to the accidental release of anhydrous ammonia from pressurized containers, UKAEA Report SRD R150, 1979.
37 Railroad Accident Report; Chicago, Burlington and Quincy Railroad Company Train 64 and Train 824 derailment and collision with tank car explosion, Crete, Nebraska, February 18, 1969, US National Transportation Safety Board Report Number NTSB-RAR-71-2, 1971.
38 R.J. Sergeant and F.E. Robinett, An experimental investigation of the atmospheric diffusion and ignition of boil-off vapors associated with spillage of LNG, Report No. 08072-7 for American Gas Association, NY, 1968.
39 F.P. Ricou and D.B. Spalding, Measurements of entrainment by axisymmetrical turbulent jets, J. Fluid Mech., 11 (1961) 21.
40 V.O. Hoehne, R.G. Luce, and L.W. Miga, The effect of velocity, temperature, and gas molecular weight on flammability limits in wind-blown jets of hydrocarbon gases, Battelle Memorial Institute report to the API, 1970.
41 G.F. Feldbauer, W.G. May, J.J. Heigl, W. McQueen, and R.R. Whipp, Spills of LNG on water-vaporization and downwind drift of combustible mixtures, ER&E Report EE.61E.72, 1972.
42 R. Humbert-Basset and L. Montet, Dispersion dans l'atmosphere d'un nuage gazeux forme par epandage de G.N.L. sure le sol, Third International Conference on Liquefied Natural Gas, Washington, D.C., 1972.
43 D.N. Gideon, A.A. Putnam, A.R. Duffy, Final Report on AGA Project IS-3-1, Comparison of Dispersion from LNG Spills over Land and Water, 1974.
44 LNG Safety Program Interim Report on Phase II Work, This report was written by personnel of Battelle Columbus Laboratories and published by the American Gas Association, 1974.
45 A. Kneebone and L.R. Prew, Shipboard Jettison Tests of LNG onto the Sea, Proc. 4th Int. LNG Conf., Amsterdam, 1974.
46 R.P. Koopman, B.R. Bowman, and D.L. Ermak, Data and calculation of dispersion on 5 m^3 LNG spill tests, Lawrence Livermore Laboratory Report UCRL-52876, 1979.
47 C.H. Buschmann, Experiments on the dispersion of heavy gases and abatement of chlorine clouds, Fourth Int. Symp. on Transport of Hazardous Cargoes by Sea, Jacksonville, Florida, 1975.
48 P.H.M. te Riele, Atmospheric dispersion of heavy gases emitted at or near ground level, 2nd Int. Sym. on Loss Prevention and Safety Promotion in the Process Industries, Heidelberg, F.R.G., 1977.
49 D.S. Burgess, J.N. Murphy, and M.G. Zabetakis, Hazards of LNG spillage in marine transportation, US Bureau of Mines, NTIS AD-705078, 1970.
50 D.S. Burgess, J. Biardi, and J.N. Murphy, Hazards of spillage of LNG into water, U.S. Bureau of Mines Report No. 4177, 1972.

51 J.A. Fay and D.H. Lewis, The inflammability and dispersion of LNG vapor clouds, Fourth Int. Symposium on Transport of Hazardous Cargoes by Sea and Inland Waterways, Jacksonville, Florida, 1975.
52 H.J. Nikodem et al., Risk assessment study for the Harbour of Gothenburg, Prepared for the Swedish Energy Commission, Stockholm, Sweden, Rep. No. BF-R-63.371-1, 1978.
53 H.J. Nikodem et al., Risk assessment study for an assumed LNG terminal in the Lysekil area, Prepared for the Swedish Energy Commission, Stockholm, Sweden, Rep. No. BF-R-31.109-1, 1978.
54 R.A. Cox and D.R. Roe, A model of the dispersion of dense vapour clouds, Proc. 2nd Int. Symp. on Loss Prevention and Safety Promotion in the Process Industries, Heidelberg, F.R.G., 1977.
55 G.D. Kaiser and B.C. Walker, Releases of anhydrous ammonia from pressurized containers, Atm. Env., 12 (1978) 2289.
56 J.A. Havens, Development of vapor dispersion models for non-neutrally buoyant gas mixtures, Progress Report to the U.S. Coast Guard DTCG 23-80-C-20029, 1981.
57 J.S. Puttock, D.R. Blackmore and G.W. Colenbrander, Field experiments on dense gas dispersion, J. Haz. Mat., 6 (1982) 13—41.
58 R.P. Koopman, R.T. Cederwall, D.L. Ermak, H.C. Goldwire, Jr., W.J. Hogan, J.W. McClure, T.G. McRae, D.L. Morgan, H.C. Rodean and J.H. Shinn, Analysis of Burro series 40 m^3 LNG spill experiments, J. Haz. Mat., 6 (1982) 43—83.
59 W.E. Mott, M. Gottlieb, and H.F. Walter, LNG research — The questions to be answered, AGA Transmission Conference, Atlanta, Georgia, May 1981.
60 A.P. van Ulden and B.J. de Haan, Two-dimensional unsteady gravity currents. 12th International Technical Meeting on Air Pollution Modelling and its Application, sponsored by NATO, Menlo Park, California, 1981.