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Comparison of heavy gas dispersion models for instantaneous releases*

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Abstract

In recent years several new heavy-gas dispersion codes have been developed. Some of these were specifically based on an analysis of the Thorney Island Heavy Gas Dispersion Trials, others were developed independently of these trials. A code-comparison exercise was considered to be a valuable contribution to the validation of these codes, though no direct comparison with experimental data has been made. Results for the following codes have been obtained: DENZ (a number of versions), CIGALE3, DEGADIS, DRIFT, EOLE, GASTAR and SLAB. Also, results from the Britter and McQuaid Workbook (BMW) have been included. Twenty-five cases have been considered; five release conditions in five meteorological conditions. All the releases are isothermal and near-instantaneous, with an initial gas density twice that of air. The most significant finding from this work is that there are still substantial differences between model codes. The major differences occur for releases at low wind speed, in Pasquill F stability and with a large roughness length. It is precisely for these conditions that experimental data are lacking. No statement can be made regarding which model is 'best', since no comparison with experimental data has been made. The question of independent model evaluation is an important one and is being addressed elsewhere.

1. Introduction

The CEA/UKAEA Exchange Agreement on External Events to nuclear power plant enables information on various topics that impinge upon the

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safety of nuclear power plant to be exchanged between the participating bodies (not solely comprising the CEA and AEA). One of the technical sub-committees of the Exchange Agreement, namely that on Gas-cloud Formation and Dispersion, comprises representatives from SRD, British Gas, CEGB, NNC, HSE, Gaz de France, CEA (Commissariat à L'Ènergie Atomique) and EdF (Électricité de France). The purpose of the committee is to foster collaborative projects and information exchange on various aspects of gas dispersion and source term work.

Following the Second Symposium on Heavy Gas Dispersion Trials at Thorney Island held in Sheffield in September 1986, it was apparent that several new heavy-gas dispersion codes were coming into use by members of the Exchange Agreement. These were either developed independently of the Thorney Island trials (namely, SLAB by Ermak and Chan [1] and DEGADIS by Havens and Spicer [2]), or were specifically based on analysis of the Thorney Island results (for example CIGALE2 by CEA (Crabol et al. [3]), and DRIFT by SRD (Webber et al. [4])). As there are a variety of ways of interpreting the Thorney Island trials (see the proceedings of the two symposia, edited by McQuaid [5, 6]), there may well be significant differences in the results of codes even for simulations within the scope of the trial conditions. A code-comparison exercise was therefore considered to be a valuable contribution to the validation of these codes. Moreover, there are different ways of optimising the parameters in the models and these differences may well be magnified when the models are extrapolated to different conditions.

Four major parameters of relevance to simulating real releases are the initial bulk Richardson number, the ratio of roughness length to cloud height, the maximum Richardson number at which top entrainment becomes important and the initial aspect ratio (height/length) of the cloud. While comparison of the codes will be useful to individual developers in detecting possible deficiencies, the major result of the comparison should be quantification of the uncertainty remaining even after careful analysis of the field trial results. Note that the comparison is between codes only; the codes have not been evaluated against experimental data. For an example of the latter, see Hanna et al. [7].

Results for the following codes have been obtained; SRD DENZ (Fryer and Kaiser [8]), HSE DENZ, HSE DENZ with the Wheatley [9, 10] cloud advection speed model, CEA CIGALE3, DEGADIS[1] and the Gaz de France code, EOLE (Girard et al. [12]), DRIFT (although DRIFT was under development at the time of the exercise, the instantaneous, isothermal model was considered to have stabilised; version 0.45 was used), GASTAR (developed by R.E. Britter of Cambridge Environmental Research Consultants Ltd. (CERC)) and SLAB (developed by D.L. Ermark et al. at Lawrence

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[1] Several of the values of the variables required in the detailed comparison are not included in a DEGADIS output file. Hence, a separate post processor was written to obtain these values from the standard output file. The choice of definition of some of these (cloud averaged concentration and position of the cloud's centroid) are somewhat subjective. See Mercer et al. [11] for a detailed account.

Livermore National Laboratory [1]). While not a 'code' in the accepted sense, the Workbook on the Dispersion of Dense Gases (Britter and McQuaid [13]) has also been used.

The results herein are presented graphically. All the results are on floppy disk so that further quantitative analysis could be carried out should this be deemed worthwhile.

2. Specification of the cases

A summary of the cases considered is given in Table 1. All cases have initial gas density twice that of air. Five meteorological conditions were considered: $U_{10}=1$ m/s, 2 m/s, 4 m/s, 8 m/s in neutral stability (Pasquill D); $U_{10}=1$ m/s in stable conditions (Pasquill F); where U_{10} is the wind speed at a height of 10 m.

For each of the five meteorological conditions there were five release conditions. The first two were an idealised Thorney Island-type release (i.e. isothermal and near-instantaneous in the form of a right circular cylinder) with two different roughness lengths, $z_0=0.01$ m and $z_0=0.3$ m (corresponding to open grassland and agricultural areas, respectively). The initial volume, V_0 was 2000 m^3, with initial height H_0 and radius R_0 equal to 13 m and 7 m, respectively; giving an initial aspect ratio, $H_0/2R_0$ approximately equal to one. To explore the effect of aspect ratio in isolation, the third case was chosen to have $V_0=2000$ m^3 and $R_0=24$ m and $z_0=0.01$ m. This gives an aspect ratio of 0.023 instead of 0.93 as in the first two release conditions. The last two release conditions can be regarded as idealisations of a release of the order of hundreds of tonnes, as a low-lying cloud (as from pool boil-off). This tests the result of moving to top entrainment at higher Richardson numbers, and also the influence of roughness length on low-aspect-ratio releases. It scales-up from the Thorney Island release by a linear dimension of 5, giving a volume

TABLE 1

Comparison of heavy-gas dispersion box models for instantaneous releases. Total 25 cases identified with letters from A to Y

Volume (m^3)	Radius (m)	Roughness length (m)	Wind speed (m/s) at 10 m and stability class				
			1		2	4	8
			D	F	D	D	D
$2.00+10^3$	7	0.01	A	B	C	D	E
		0.3	F	G	H	I	J
	24	0.01	K	L	M	N	O
$2.5+10^5$	120	0.05	P	Q	R	S	T
		1.5	U	V	W	X	Y

$V_0 = 250{,}000\,\mathrm{m}^3$ and $R_0 = 120\,\mathrm{m}$ with an aspect ratio of 0.023 again. The roughness length was also scaled up to 0.05 m and 1.5 m to give the last two of the five sets of release conditions.

It was recognised that there may be difficulties in computing low-windspeed cases with large surface roughness, if the cloud height gets close to about twice z_0, and so some results may be missing in this corner of the matrix. (In a number of models of the type considered in this report, the cloud advection speed is taken to be the ambient wind speed at some fraction (typically one half) of the cloud height.) A worthwhile result of the comparison exercise is to bring such problems out into the open.

It was also regarded as important to specify precisely the output required on which to base the comparison. It is highly desirable to have output of numerical values at identical times and locations, so that a quantitative assessment of model differences can be made. In order to highlight differences in the formulation of the models, the quantities should include all the basic working parameters of the models, i.e. cloud speed, length, width and (mean) cloud concentration. Also while variations of these quantities with time are more fundamental physically, variations with distance from the source are more directly useful for practical purposes. So for each case, it was decided to compare predictions for the cloud centroid speed U_C, the cloud width W and length L and the mean ground-level cloud concentration C. In the event, the comparison was based on the cloud volume-average concentration, except for the results from the Britter–McQuaid Workbook. These are estimates, from experimental data, of the ensemble mean of the maximum of the short-time averaged concentration-time histories at ground level; see Britter and McQuaid [13]. In the case of models with a generalised concentration profile, the cloud outline is taken as the contour of one-tenth the central maximum value.

These quantities were required at five standard distances and five standard times. The distances to the cloud centroid are 30 m, 100 m, 300 m, 1000 m and 3000 m along the centreline from the source for release volumes of $2000\,\mathrm{m}^3$. For the volume of $2.5 + 10^5\,\mathrm{m}^3$, these distances are increased by a factor of five to range from 150 m to 15 km. For the standard distances, the times at which the maximum concentration is reached (the arrival time in the case of top hat profiles) were also required. The standard times for output are obtained by dividing the standard distances by $0.8U_{10}$.

Note that the comparison exercise does not involve any direct use of the Thorney Island data as this is outside the scope of the present exercise as outlined in the Introduction.

3. Results presented herein

The results of the comparison exercise are extensive. The full set of results is published in Mercer et al. [11]. For the purposes of this paper, the results for two release conditions only are given.

The chosen cases are: case I, a Thorney Island scale release in neutral stability with U_{10} equal to 4 m/s and case Q, a scaled-up small aspect ratio release in F stability and with U_{10} equal to 1 m/s.

For these two cases, the following quantities are presented graphically: (a) cloud-average concentrations as a function of distance and of time; (b) cloud widths as a function of distance and time; and (c) position of the cloud centroid (on the ground) as a function of time.

The following comments are appropriate.

(a) In the box-model formulation, in the dense regime, the cloud-average concentration is, by definition, the uniform concentration throughout the cloud volume, i.e. the 'top-hat concentration'. In the passive regime, however, the determination of a cloud-average concentration presents some difficulty, because the cloud boundary is not delineated. This is because most models fit a Gaussian curve to the concentration distribution across the cloud (horizontally and vertically) after the cloud is deemed to be passive. Since the Gaussian curve extends out to infinity, some arbitrary definition of the cloud boundary has to be made. The usual choice is to define the cloud outline in terms of the '10% edge'; for a Gaussian form, the width is about $4\sigma_Y$. Thus, for a nominally cylindrical cloud, in any horizontal slice the edge of the cloud is where the concentration has fallen to 10% of that on the axis. The height of the cloud is the distance along the vertical axis to where the concentration is 10% of its value on the ground. This procedure is used in the SRD and HSE versions of DENZ; it allows the determination of the cloud-average concentration in terms of the ground-level, cloud centre value, see Mercer et al. [11], for a detailed description. Furthermore for other codes, such as DEGADIS, using a combination of a box of uniform concentration with an outlying region containing profiles of different shapes, the calculation of a cloud-averaged concentration is even more complicated.

It is clear that the cloud boundary so defined is not the same as the contour of one-tenth the central maximum value on the ground. Under the definition used in DENZ, the concentration at the 'top-corner' of the cloud is 1% of the central maximum value. The definition of the cloud-average concentration may differ from model to model. This will be a factor in explaining differences between model results in the passive regime.

(b) When using a dispersion model within a risk assessment procedure, the cloud dimensions (on the ground) as well as concentration are important since these, for a toxic substance, determine the dose. (See for example, Nussey et al. [14].) The cloud width was therefore included in the specification. In most of the 'early' codes, the cloud is modelled as a right circular cylinder throughout its motion. In the more recent models (e.g. DRIFT, GASTAR and SLAB), differences between lateral and longitudinal spreading/diffusion is allowed for, resulting in the cloud length becoming greater than the cloud width at some stages. While results on cloud length are available, they have not been included on the graphs.

(c) One of the unresolved problems in formulating a box-model for dense-gas dispersion is the prescription of the cloud advection speed. Differences between models in this respect will be apparent from these presentations.

4. Discussion of the results

Graphs of the three quantities discussed above have been prepared for all 25 cases, specified in Table 1. Here, results for cases I and Q only are presented. In any event, for most of the models, a complete set of results for the cases U, V, W, X and Y is not available because the cloud height gets close to the roughness length, z_0, which results in the computations being terminated. That this might happen was anticipated when the specification for the cases was drawn up.

(i) For the set of results of cloud-average concentration as a function of downwind distance, for the 2000 m^3, near unity aspect ratio, low roughness releases (cases A to E), there are fairly substantial differences between the models. In the dense regime, with some exceptions, these are by factors of up to about 5. The results from the Britter–McQuaid Workbook (BMW), on the whole, lie reasonably within the body of the data from the model codes. This is rather surprising since the BMW correlations represent ensemble averages of the maximum in short-time averaged (0.6 s) data. On the other hand, the BMW correlations are based on results from experiments on releases at near-unity aspect ratio and small roughness length.

For the set of results at the larger roughness of 0.3 m, (cases F to J, see Fig. 1(a) for case I) still considering the dense regime, similar remarks may be made to those above. Note now that since the BMW correlations do not take into account roughness length (nor atmospheric stability), the effect of increasing the roughness length is apparent. The BMW estimates are now almost an upper bound.

For the set of results at the lower aspect ratio ($H_0/2R_0 = 0.023$) with $z_0 = 0.01$ m (cases K to O), the results are more variable, particularly at low wind speeds where the differences are about an order of magnitude or more. It is noteworthy that the BMW results still lie reasonably within the body of data from the model codes, even though the initial aspect ratio is much less than unity. This may indicate, for these releases, that the aspect ratio is less important than surface roughness.

Similar remarks may also be made for the large volume releases with small aspect ratio ($H_0/2R_0 = 0.023$) and roughness length scaled up to 0.05 m (cases P to T, see Fig. 1(b) for case Q). Now, however, there are some interesting contrasts with the BMW results. At low wind speeds the BMW results lie towards the bottom of the body of the other data, but as the windspeed increases, the BMW results lie more within the body of the other data.

For the companion set of results at the scaled-up roughness length of 1.5 m, cases U to Y, some models failed to run at low wind speeds; in particular, DENZ

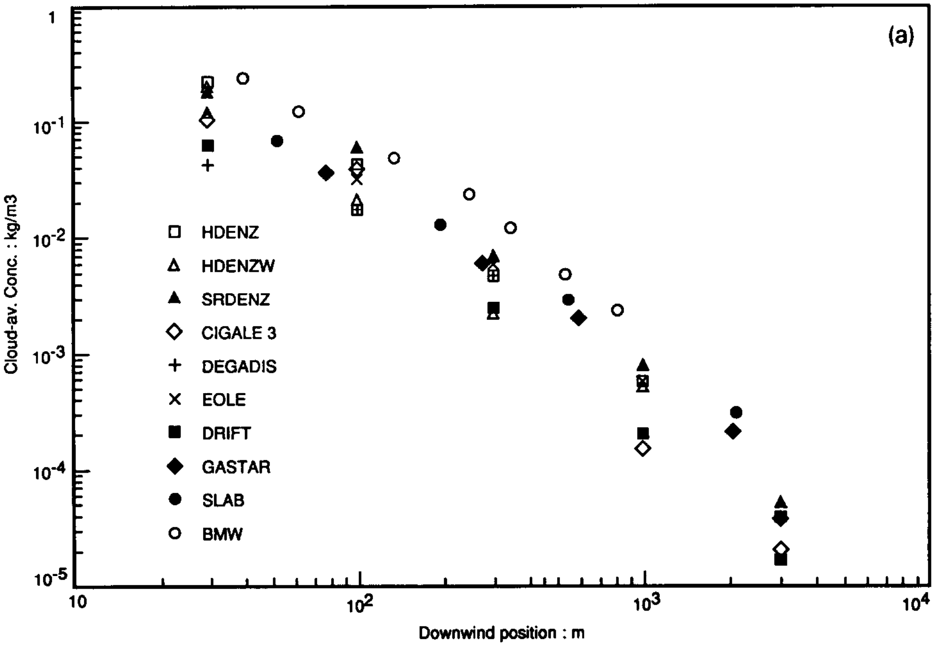

Fig.1a - Cloud-av. Conc., Case I Vo=2000m3 Ro=7m Zo=0.30m U10=4m/s Pasquill D

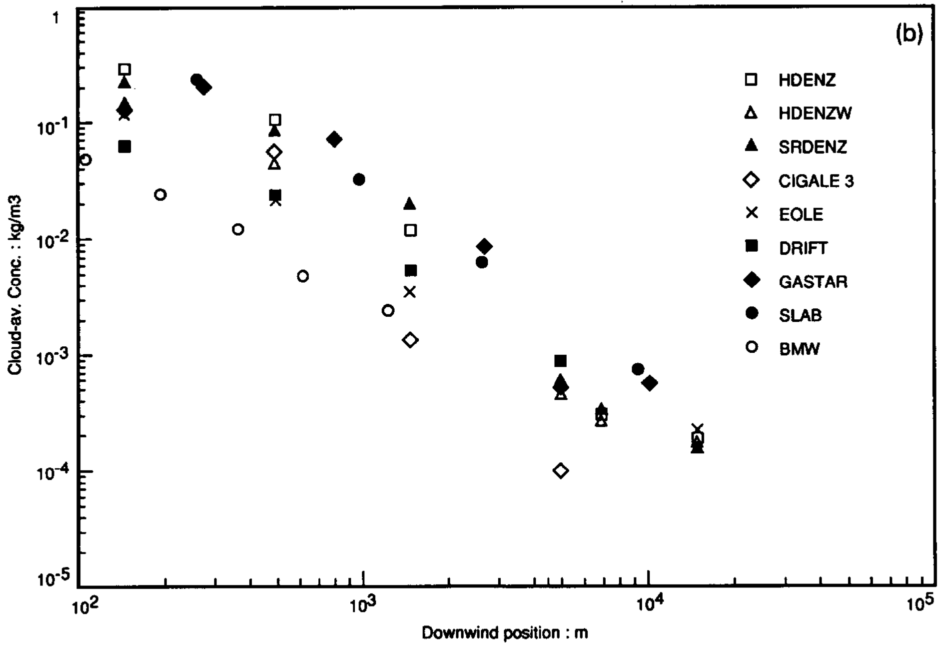

Fig.1b - Cloud-av. Conc., Case Q Vo=2.5E+5m3 Ro=120m Zo=0.05m U10=1m/s Pasquill F

and its derivatives. The reason for this is that in these models, the cloud advection speed is taken to be that of the ambient wind at half the cloud height. Should the cloud height fall to below twice the roughness length, the calculation breaks down since the logarithmic wind profile is only valid for $z > z_0$.

A noteworthy feature of the large volume releases is that the differences between models are comparable to those for the 2000 m^3 releases. This suggests that the scaling properties of the models are similar.

On the whole, the differences are not as great when the concentrations are presented as a function of time, see Figs. 2(a) and (b). This indicates that the cloud advection speed is a major factor in the differences shown in the first set of figures.

In the passive regime, with two exceptions, the models compare quite well, to within a factor of less than two. The exceptions are DEGADIS at low wind speeds and CIGALE3 also in low wind speed. The reason that the results for CIGALE3 differ in the passive regime is because CIGALE3 uses the Doury scheme for the diffusion coefficients, whereas the other models use the Pasquill–Gifford scheme or similar scheme; see the Appendix. The differences between the schemes are discussed by Doury [15, 16] and by Wheatley et al. [17].

The differences do not appear to depend on scale or roughness length, with the exception of the results from DRIFT. For both the 2000 m^3 and large scale releases at the greater roughness lengths, the predicted concentrations from DRIFT tend to be lower than those from the other models.

Corresponding remarks may be made for the set of results of concentration as a function of time, in the passive regime.

(ii) For the results for cloud width as a function of downwind distance, for the 2000 m^3 and large volume, near-unity aspect ratio releases (cases A to J and P to Y, see Figs. 3(a) and (b) for cases I and Q), with some exceptions, the differences between the model codes are no more than a factor of two. The exceptions are the CEA results in the passive regime in low wind speed (for the reasons outlined above) and the results for case G, namely for the large roughness at a low wind speed in Pasquill category F, where in the passive regime the differences between the codes approach a factor of three (excluding the CEA points) and are beyond this factor with the CEA points (see the Appendix).

In the dense regime, the BMW results are well within a factor of two of the model codes. In the passive regime however, except at the largest wind speed of 8 m/s, the BMW results are consistently greater than the other model codes (except CEA in low wind speed).

Similar remarks may be made for the low aspect ratio releases, cases K to O, but with the differences between model codes now a little greater.

Again, it is noteworthy that the differences between models is comparable for both the 2000 m^3 and large volume releases.

The differences are less marked when the presentation is in terms of travel time (see Figs. 4(a) and (b) for cases I and Q) particularly at the higher wind speeds; supporting the statement regarding the cloud advection speed made in the previous section.

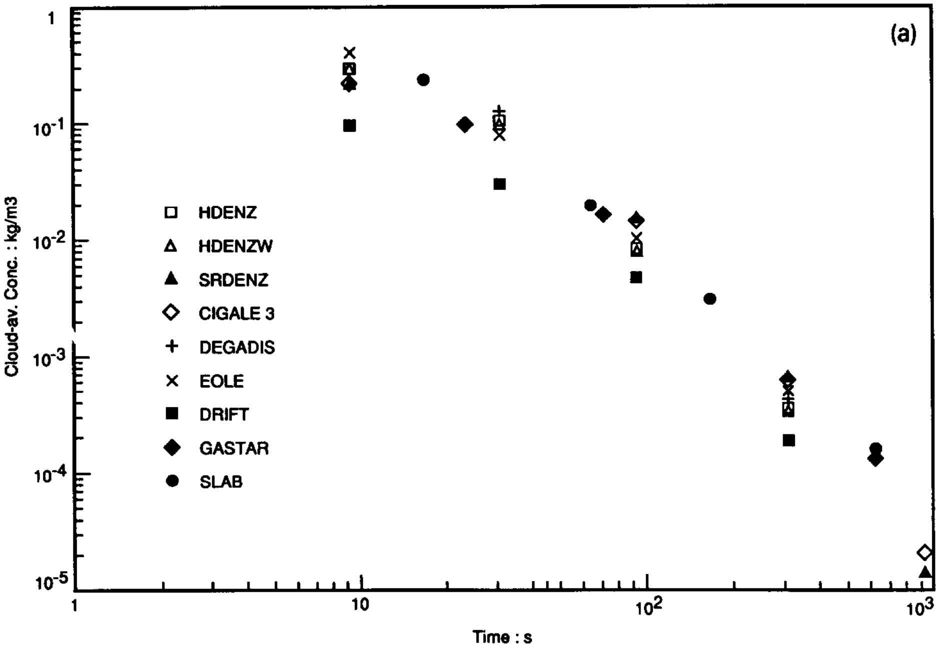

Fig.2a - Cloud-av. Conc., Case I Vo=2000m3 Ro=7m Zo=0.30m U10=4m/s Pasquill D

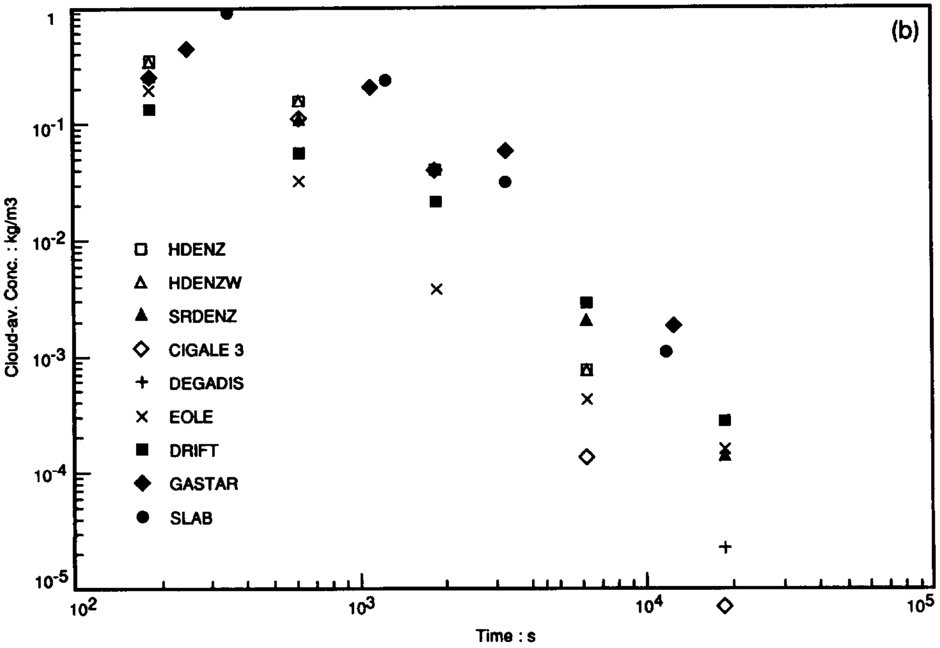

Fig.2b - Cloud-av. Conc., Case Q Vo=2.5E+5m3 Ro=120m Zo=0.05m U10=1m/s Pasquill F

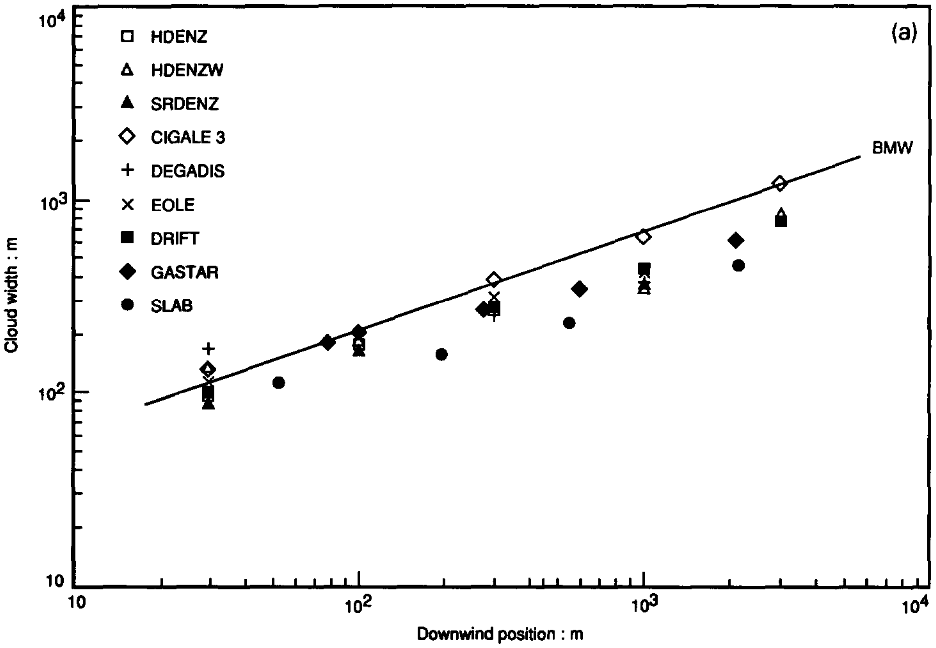

Fig.3a - Cloud width, Case I Vo=2000m3 Ro=7m Zo=0.30m U10=4m/s Pasquill D

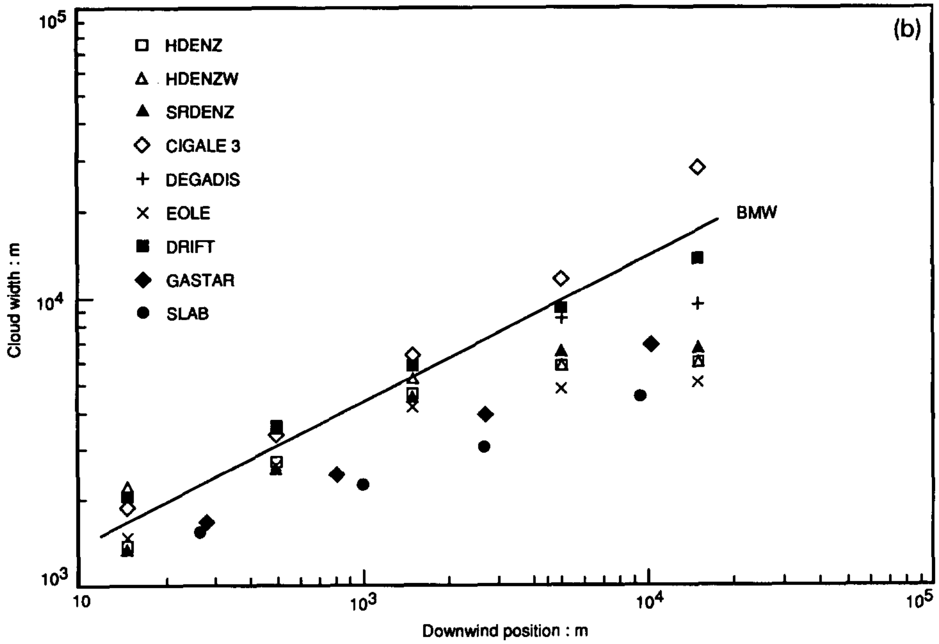

Fig.3b - Cloud width, Case Q Vo=2.5E+5m3 Ro=120m Zo=0.05m U10=1m/s Pasquill F

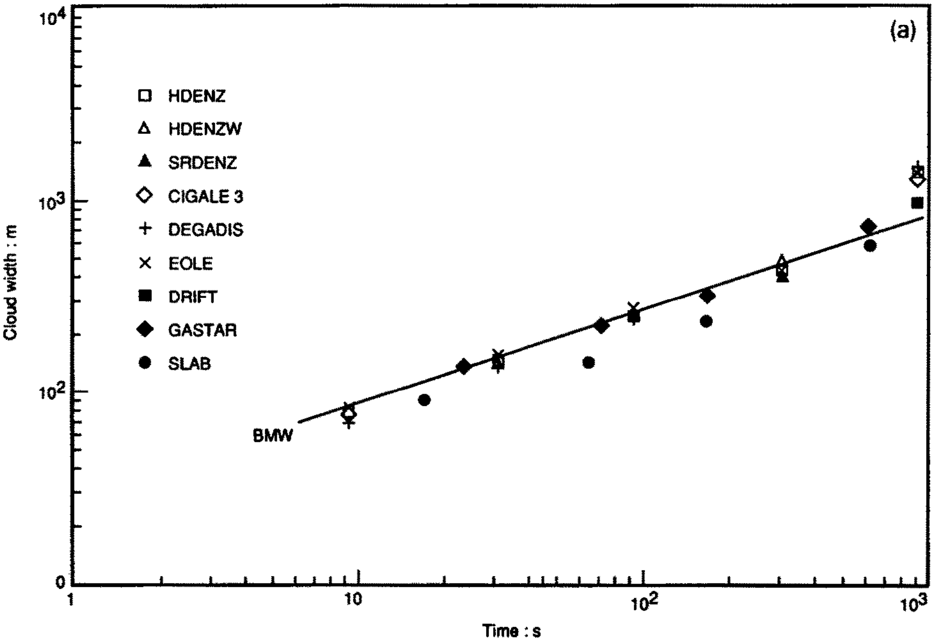

Fig.4a - Cloud width, Case I Vo=2000m3 Ro=7m Zo=0.30m U10=4m/s Pasquill D

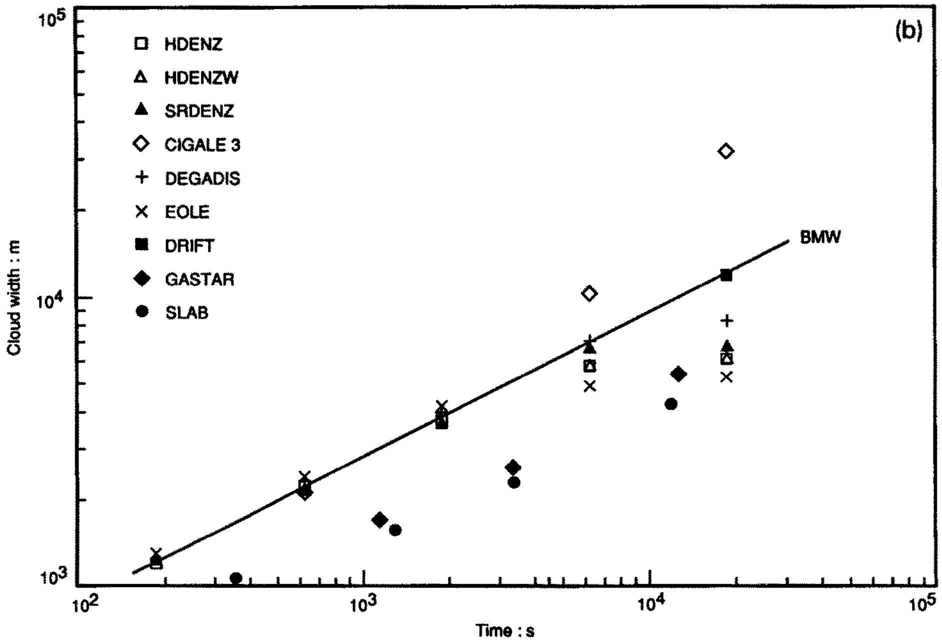

Fig.4b - Cloud width, Case Q Vo=2.5E+5m3 Ro=120m Zo=0.05m U10=1m/s Pasquill F

(iii) The cloud centroid position (on the ground) as a function of travel time is shown in Fig. 5. (That the results have a step-like character is due to having combined the results for times to reach the standard distances with the distances reached at the standard times.) The cloud advection speed in the Britter–McQuaid Workbook is taken to be $0.4U_{\text{ref}}$. Here U_{ref} is taken to be U_{10}, so that the cloud centroid position is simply given by $x=0.4U_{10}t$; this relationship is represented by the lines shown on this set of figures. (Note that for more complex codes such as DEGADIS, the definition of the cloud centroid is not straightforward; see Mercer et al. [11].)

For the 2000 m^3 near unity aspect ratio releases, cases A to J, at low wind speeds the differences between model codes are about a factor of three at short travel times (in the dense regime) decreasing to a factor of about 1.5 at long travel times (in the passive regime). At the higher wind speeds, see Fig. 5(a) for case I, these factors increase to about 5 and 2, respectively. Two exceptions are cases B and G for releases in Pasquill F stability; the differences between model codes now do not decrease with increasing travel time.

There appears to be little or no effect of increasing the roughness length on the results at short travel times, but the differences at long travel times are greater than for the small roughness length cases. This is particularly so for the release at 1 m/s in Pasquill F stability, case G. At long travel times, the model codes now differ by a factor of four.

For the 2000 m^3, low aspect ratio releases, cases K to O, the differences between model codes are now greater. At short travel times, the factors range from 5 at the low wind speed to about 20 at the highest wind speed. At long travel times, there are differences of about a factor of 2, with no dependence on wind speed. An exception is the release in F stability, case L, where, at long travel times, the factor is about 3.

For the large volume, low aspect ratio releases, at the scaled up roughness of 0.05 m, case P to T, see Fig. 5(b) for case Q, the results are comparable to those from the companion set, K to O. It is noteworthy that for the large volume releases, at short travel times, the differences are less than those for the 2000 m^3 releases but at long travel times, the converse is true.

Note again that for the release in F stability, case Q, at long travel times, the model codes now differ by a factor of 6 to 7.

For the large volume releases at the large roughness length, cases U to Y, while it needs to be borne in mind that some models failed to run for some of these cases, similar remarks still apply as for the companion set F to J.

On the whole, the results from the codes tend to start below and end above the nominal line, $x=0.4U_{10}t$. This is reasonable as the cloud is accelerated as it gains in height.

5. Discussion

In general, the differences between the model's predictions of concentration and cloud width are within factors of 3 to 5. There are more substantial

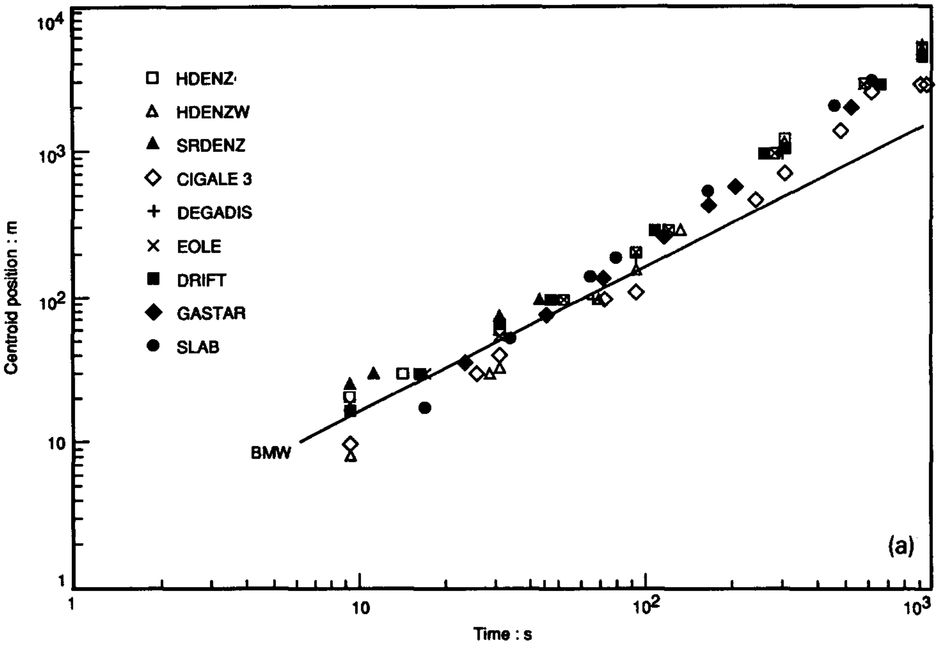

Fig.5a - Centroid position Case I Vo=2000m3 Ro=7m Zo=0.30m U10=4m/s Pasquill D

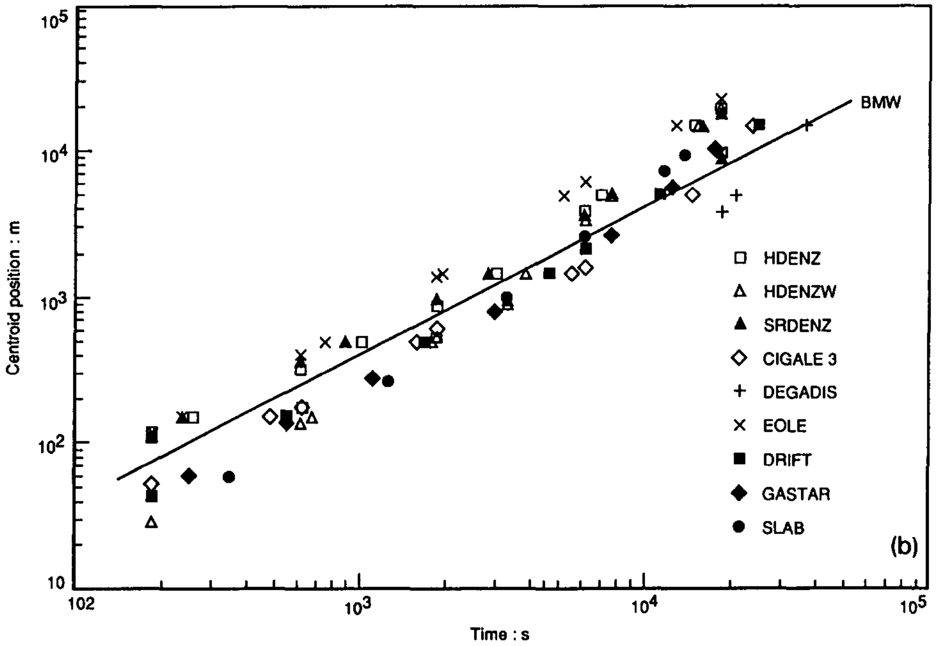

Fig.5b - Centroid position Case Q Vo=2.5E+5m3 Ro=120m Zo=0.05m U10=1m/s Pasquill F differences for releases at low wind speed and large roughness length. There are also substantial differences in the prediction of cloud centroid position for low aspect releases at short travel times.

However, since one of the main uses of models is in quantified risk assessment (QRA), the question arises whether such factors are significant for QRA. This question has been addressed by Nussey et al. [14]. One of the conclusions of this paper was that because of trade-offs between concentration levels and cloud/plume dimensions and cloud passage times, models that differ by factors of 2 or 3 in their predictions of maximum concentration, can — when used within a risk assessment tool — lead to similar predicted levels of risk.

6. Conclusions

The most significant finding from the code comparison exercise is that there are still substantial differences between model codes, even when these codes have been parameterised using essentially the same experimental data. It should be noted that no statement can be made regarding which model is 'best', since no comparison with experimental data has been made. Of course, the model developers will have carried out such comparisons. The question of independent model evaluation is an important one and is being addressed elsewhere.

The major differences occur for releases at a low wind speed, in Pasquill F stability and with a large roughness length. It is precisely for these conditions that experimental data is lacking. An important factor here is the modelling of the cloud advection speed.

On the whole, the differences between model codes for the large volume releases are not greater than those for the $2000\,m^3$ releases. This suggests that the scaling properties of all the models are essentially similar.

While there are substantial differences between model codes, this does not necessarily mean that, when used in risk assessment programmes, the differences in risk levels will be of the same order. Since the individual risk at a point depends on both the concentration distribution and on the cloud dimensions, there are 'trade-offs' between these two aspects which result in the differences in the risk being much less than the differences in the concentration and cloud dimensions themselves. Also, low wind speeds with Pasquill F stability is an uncommon weather condition and not likely to give the greatest hazard ranges. (Of course, this argument is invalid for the important case where one model predicts zero risk at a particular distance and another predicts a finite risk.) Therefore, it is possible that the risk implications of variability of factors of 2 or 3 in predicted dispersion behaviour are not substantial. It may be more important to be satisfied that the physical modelling in the various codes is reasonable and the limits of applicability clearly understood by the users.

Acknowledgements

The author is grateful to all the participants for providing the results from their model codes and to Dr R.E. Britter and Dr. D.L. Ermak for making available the codes GASTAR and SLAB, respectively.

Appendix

Comments from CEA

The CEA results have been obtained with the code CIGALE3. These results are, in the gravity phase, comparable to those of the other codes, and, in the passive phase, notably different essentially for low wind speed conditions (cases of wind speed of 1 m/s or 2 m/s in the present exercise). The main reason is the use in the code CIGALE3 of Doury's standard deviations while the other codes use, in the passive regime, standard deviations comparable to those of the Pasquill–Gifford scheme. One of the main differences between the two schemes is that Doury's parameters are dependent on the travel time of the puff while the P–G parameters depend on the travel distance. It leads to the fact that, with Doury's parameters, for low wind speed, the concentrations, at given distances downwind, are lower than with a higher wind speed while it is the contrary with the P–G parameters. Another difference is that Doury's horizontal standard-deviations are independent of the atmospheric stability while the P–G standard-deviations decrease as the atmospheric stability increases. Finally, in Doury's scheme in contrast to the P–G scheme, the influence of ground roughness is assumed to be negligible.

Note also that the CEA results in this report are presented as those of the latest version of CIGALE3. In fact, when the exercise was set up in 1986, CEA was developing version 2 of CIGALE and the first results sent at the time were those from this version of the code. Since then, the new version CIGALE3 has been developed. In order to avoid a complete revision of the graphs which were already drawn, the values obtained with the old version were not modified when the differences were small compared with the new version.

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