ELSEVIER

Journal of Hazardous Materials A103 (2003) 1–10

Journal of Hazardous Materials

www.elsevier.com/locate/jhazmat

Heavy gas dispersion: integral models and shallow layer models

Robin K.S. Hankin*

School of Geography and Environmental Science, The University of Auckland, Private Bag 92019, Glen Innes, Auckland, New Zealand

Received 3 January 2003; received in revised form 5 January 2003; accepted 21 June 2003

Abstract

Integral models for heavy gas dispersion approximate a dispersing cloud in terms of a small number of variables; each of these is ultimately a function of an independent variable which is usually time (instantaneous releases) or downwind distance (continuous releases).

This type of model is used almost exclusively in risk assessment [HSE's risk assessment tool, RISKAT, in: Major Hazards: Onshore and Offshore, October 1992, pp. 607–638; Ann. Rev. Fluid Mech. 21 (1989) 317], but many distinct integral models exist. The code comparison exercise of Mercer et al. [CEA/AEA exchange agreement on external event. Comparison of heavy gas dispersion models for instantaneous releases: final report, Technical Report IR/L/HA/91/6, Health and Safety Laboratory, Sheffield, June 1991; J. Hazard. Mater. 36 (1994) 193] presented the results from a number of integral models in a common format; Mercer found that the range of predictions for some scenarios exceeded three orders of magnitude.

Here, the TWODEE shallow layer model [J. Hazard. Mater. 66 (3) (1999) 211; J. Hazard. Mater. 66 (3) (1999) 227; J. Hazard. Mater. 66 (3) (1999) 239] is added to Mercer's code comparison exercise. The physical assumptions used in shallow layer models differ profoundly from those used in integral models and the implications of these differences for risk assessment are discussed.

TWODEE was used to simulate four representative cases considered by Mercer. In terms of cloud averaged concentration (CAC) vs. centroid position, the present model gave predictions that were consistent with the integral models used by Mercer.

As the model neglects horizontal diffusion for passive clouds, overprediction at large downwind distances was expected, but not generally observed.

Keywords: Heavy gas dispersion; Shallow layer model; Integral models; Model comparison

* Present address: Southampton Oceanography Centre, University of Southampton, Waterfront Campus, European Way, Southampton SO14 3ZH, UK.
E-mail address: r.hankin@soc.soton.ac.uk (R.K.S. Hankin).

0304-3894/$ – see front matter © 2003 Elsevier B.V. All rights reserved.
doi:10.1016/S0304-3894(03)00219-X

1. Introduction

The assessment of off-site risk near major hazard sites is typically carried out using tools such as RISKAT [1]. The consequence analysis carried out by such tools includes simulations of heavy gas dispersion which are typically carried out by integral models [1,2]. An integral model is one which solves only ordinary (as opposed to partial) differential equations [8].

A large number of distinct integral models for dense gas dispersion exist; amongst these, the range of predictions for some scenarios may exceed three orders of magnitude [4].

1.1. *Shallow layer models for dense gas dispersion*

Motivated by the low aspect ratio of typical heavy gas clouds, shallow layer models use depth-averaged variables to describe the flow behavior [8]. One shallow layer model is the TWODEE model of Hankin and Britter [5].

Shallow layer models for dense gas dispersion are physically realistic, computationally cheap, and suitable for use in risk assessment [8]. Britter [2] states, in a discussion of computational fluid dynamics (CFD) models for heavy gas dispersion, that shallow water models would be a “pragmatic alternative”.

The approach is thus is a compromise between the complexity of CFD models [8] and the simpler integral models. It is particularly well suited to assess the effect of complex terrain because the downslope buoyancy force is easily included, although only flat ground is considered here. Entrainment may be incorporated into a shallow layer model by the use of empirical formulae.

Shallow layer models are not without disadvantages: they need orders of magnitude more computer time to run than integral models. In a risk assessment context, shallow layer models are perhaps best used as a complement to integral modeling [8].

1.1.1. *TWODEE*

The TWODEE computer model [5–7] simulates the shallow water equations with boundary conditions which ensure a front Froude number of unity. Thus, the cloud is described in terms of depth-averaged variables which vary in (two-dimensional) space and time; the model is useful for isothermal, monophase releases.

The four variables are: cloud depth h, depth-averaged cloud density $\bar{\rho}$, and two components of depth-averaged velocity $(\bar{u}, \bar{v})$. The following relations are used for *definition* of these four depth-averaged quantities:

$$h(\bar{\rho} - \rho_a) = \int_{z=0}^{\infty} [\rho(z) - \rho_a]\,\mathrm{d}z, \tag{1}$$

$$h(\bar{\rho} - \rho_a)\bar{u} = \int_{z=0}^{\infty} [\rho(z) - \rho_a]u(z)\,\mathrm{d}z, \tag{2}$$

$$h(\bar{\rho} - \rho_a)\bar{v} = \int_{z=0}^{\infty} [\rho(z) - \rho_a]v(z)\,\mathrm{d}z. \tag{3}$$

A fourth equation is required to close the system; Hankin [8] shows that it is convenient and meaningful to specify cloud height h as that height below which 95% of the buoyancy is located, viz:

$$\int_{z=0}^{h} [\rho(z) - \rho_a]\,\mathrm{d}z = 0.95 \int_{z=0}^{\infty} [\rho(z) - \rho_a]\,\mathrm{d}z. \tag{4}$$

These depth-averaged variables evolve according to the standard shallow water equations, but with an extra term that ensures that the leading edge moves with a Froude number of unity; full details are given by Hankin and Britter [5]. The vertical profile used is not needed for the code comparison exercise presented below, because Eqs. (1)–(4) give meaningful values for h and $\bar{\rho}$ for *any* vertical profile.

Comparison between shallow layer models and integral models is thus not straightforward because of the very different representations used for the cloud.

2. The code comparison exercise of Mercer

In 1991, Mercer compared a number of heavy gas dispersion models against one another [3,4]; the work was carried out as a result of the development of a number of new dispersion codes.

The development of these codes followed the Second Symposium on Heavy Gas Dispersion Trials at Thorney Island [9]; it had become clear that significant differences in the results of codes existed, even for simulations within the scope of the trial conditions. Mercer attributed these differences to varying ways of optimizing the parameters in the models.

Mercer considered 25 cases: 5 different releases under 5 meteorological conditions (Table 1); in each case, the density of the release was twice than that of air. The comparison exercise did not involve any direct use of the Thorney Island data. Mercer's results were made publicly available and are used here.

Each of the cases A–Y have been considered by the present author [8,10] and four are selected for presentation here: cases A, E, P, and T. These cases span the range of windspeeds considered, involve only neutral stability, and had a value of z_0 compatible with the present approach. These cases were representative of the whole.

Mercer's methodology was intended for use with integral models. The present model, being a shallow layer simulation, differs considerably from the models considered by Mercer. A review of the methodology used in this paper follows.

Table 1
The 25 cases considered by Mercer

Volume (m^3)	Radius (m)	z_0 (m)	Windspeed (m/s) at 10 m and stability class				
			1; D	1; F	2; D	4; D	8; D
2×10^3	7	0.01	A	B	C	D	E
2×10^3	7	0.3	F	G	H	I	J
2×10^3	24	0.01	K	L	M	N	O
2.5×10^5	120	0.05	P	Q	R	S	T
2.5×10^5	120	1.5	U	V	W	X	Y

3. Methodology of including the present model in Mercer's code comparison

Mercer's work was carried out using integral models, in which cloud-wide averaging takes place at the modeling stage. Shallow layer simulations, not being uniform in height or density, render the concepts of 'cloud radius' and 'cloud height' not directly meaningful; but a reasonable method by which simulations may yield a 'cloud averaged concentration' (CAC) as a function of 'downwind distance' is given below.

In contrast, shallow layer simulation results are in the form of functions of two spatial dimensions and time; the outputs of interest are the depth-averaged quantities $h = h(\mathbf{x}, t)$ and $\bar{\rho} = \bar{\rho}(\mathbf{x}, t)$. Here, $\mathbf{x} = (x, y)$ is the ground position and t the time from release; an overbar denotes a depth-averaged quantity as defined in Eqs. (1)–(4).

It is not clear that 'CAC as a function of downwind distance' is meaningful in this more general context. However, it is possible to proceed by defining a buoyancy-weighted cloud centroid position vector $\mathbf{P} = \mathbf{P}(t)$ as follows:

$$\mathbf{P} \int_{\mathbf{x}:\bar{\rho}(\mathbf{x},t)>\rho_a} h(\bar{\rho} - \rho_a)\, \mathrm{d}^2\mathbf{x} = \int_{\mathbf{x}:\bar{\rho}(\mathbf{x},t)>\rho_a} h(\bar{\rho} - \rho_a)\mathbf{x}\, \mathrm{d}^2\mathbf{x}, \tag{5}$$

where $\mathrm{d}^2\mathbf{x} = \mathrm{d}x\,\mathrm{d}y$ is an infinitesimal element of area, and the cloud averaged density ρ^* satisfies

$$\rho^* \int_{\mathbf{x}:\bar{\rho}(\mathbf{x},t)>\rho_a} h\, \mathrm{d}^2\mathbf{x} = \int_{\mathbf{x}:\bar{\rho}(\mathbf{x},t)>\rho_a} h\bar{\rho}\, \mathrm{d}^2\mathbf{x}. \tag{6}$$

The definitions of h and $\bar{\rho}$ imply that ρ^* is a representative density of the cloud over points where $\bar{\rho} > \rho_a$. The cloud-averaged concentration C^* may be obtained using the equation of state.

Now, $P = |\mathbf{P}|$ is the distance of the centroid from the release point, and $C^* = C^*(t)$ is the CAC, at time t. It is thus possible to use a sequence of simulation results to give a series of Ps and C^*s, yielding $C^* = C^*(P)$, as required. Quantities such as cloud width or radius are not straightforward to define as they are used only in integral models.

Thus CAC C^* can be calculated as a function of downwind distance P. The methodology of integral models uses downwind distance (or time from release) and CAC as starting points for the rest of the model; these quantities are not used in shallow layer modelling. Here C^* and P are *calculated* from simulation outputs and this methodology is used here to include TWODEE in Mercer's code comparison exercise.

3.1. Time from release as the independent variable

Mercer also considered time from release as the independent variable (as opposed to distance). He found that differences between models were generally smaller when results were expressed against time and interpreted this in terms of differing cloud advection speeds used in the models. Such arguments are difficult to apply to TWODEE, as cloud centroid has only a restricted meaning.

TWODEE is consistent with the consensus of integral models predictions if time is used as an independent variable [8,10].

4. Results

The results that follow show predictions from TWODEE and the models considered by Mercer. Four graphs are shown; TWODEE predictions are shown in bold.

The lines in each figure were calculated by logarithmic interpolation between the points provided by Mercer; typically results from four distances were considered. Results from TWODEE are calculated in the same way, giving rise to the abrupt changes of slope.

Large values of z_0. Mercer's cases U–Y used a roughness length z_0 of 1.5 m; this corresponds to "centers of cities with very tall buildings" on flat ground [11]. For each of these cases, most of the integral models did not give results because the cloud height at early times is less than z_0. As a logarithmic velocity profile (wrongly) predicts negative windspeeds for this situation, useful models, including TWODEE, simply flag that the source terms are inconsistent with the surface roughness length.

4.1. *Case A: volume* 2×10^3 m^3*, radius 7 m, windspeed 1 m/s*

Fig. 1 shows TWODEE's predictions for case A against downwind distance from release point to cloud centroid. For distances up to $\sim 10^3$ m, TWODEE gives predictions that lie

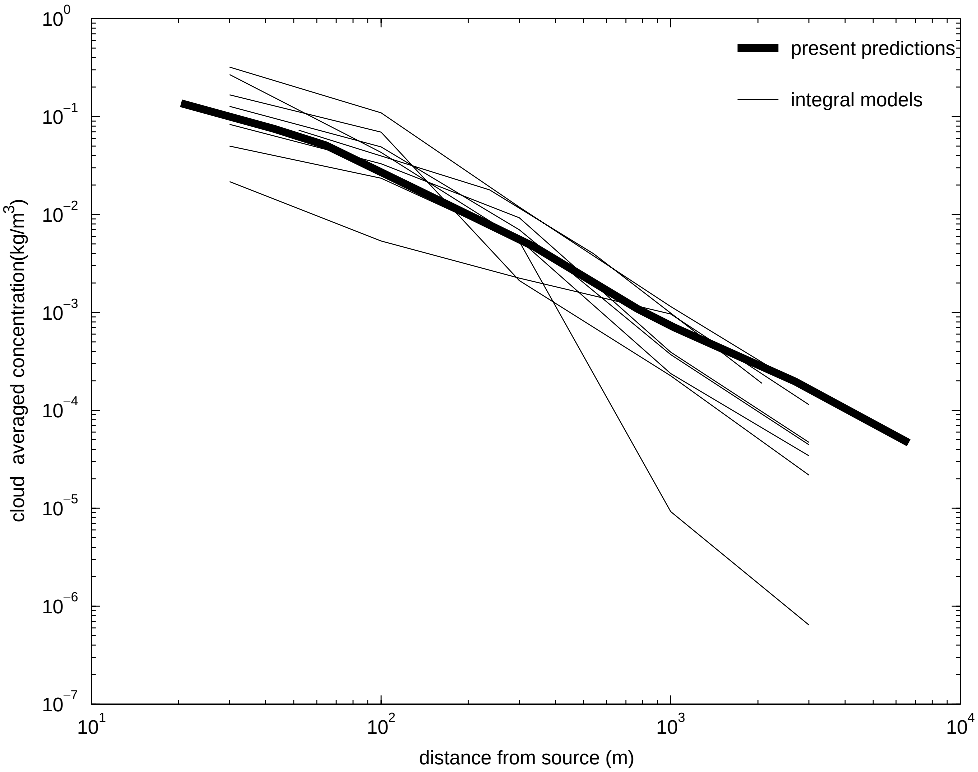

Fig. 1. CAC vs. downwind distance, case A.

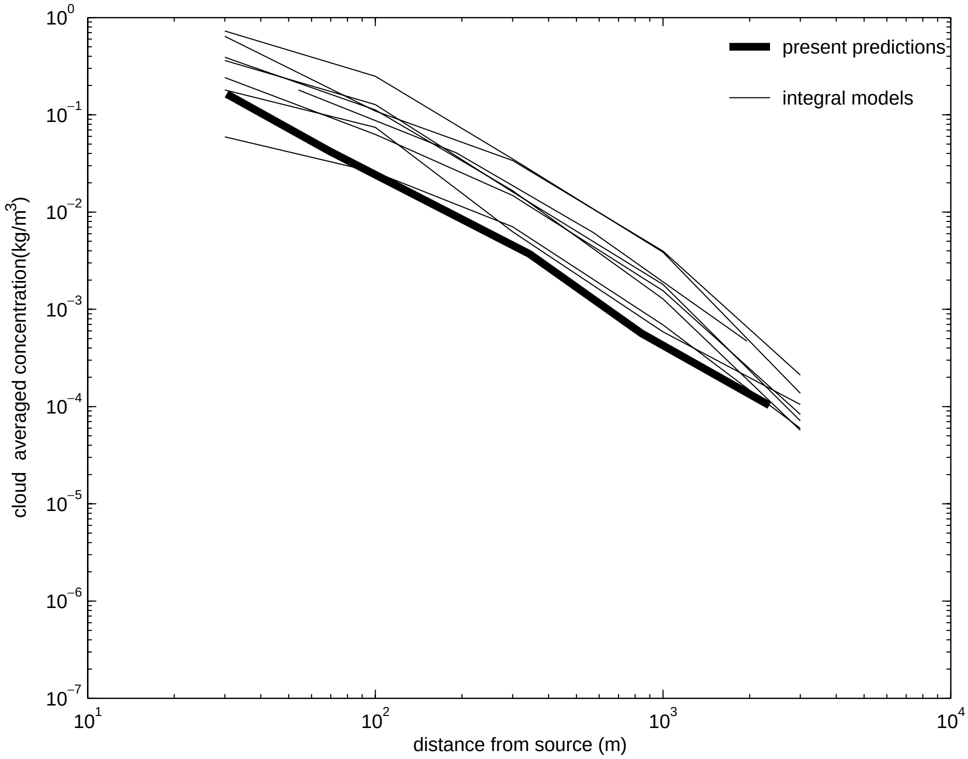

Fig. 2. CAC vs. downwind distance, case E.

within the range; at larger distances, TWODEE's predictions lie at the upper end. This figure includes one model with predictions for 3000 m an order of magnitude lower than any other model. Even without this model, however, there is a spread of a factor of $\simeq$10 at this distance.

4.2. *Case E: volume* 2×10^3 m^3*, radius 7 m, windspeed 8 m/s*

Fig. 2 shows TWODEE's predictions against downwind distance for case E. Here, TWODEE's predictions lie at the lower end of the range.

Integral models for case E agree more closely at a given distance than those for case A; this is also true for predictions at a given time. Fig. 2 exhibits a range of about an order of magnitude.

4.3. *Case P: volume* 2.5×10^5 m^3*, radius 120 m, windspeed 1 m/s*

Fig. 3 shows TWODEE's predictions against downwind distance for case P. Here, the TWODEE predictions lie at the upper end of the range.

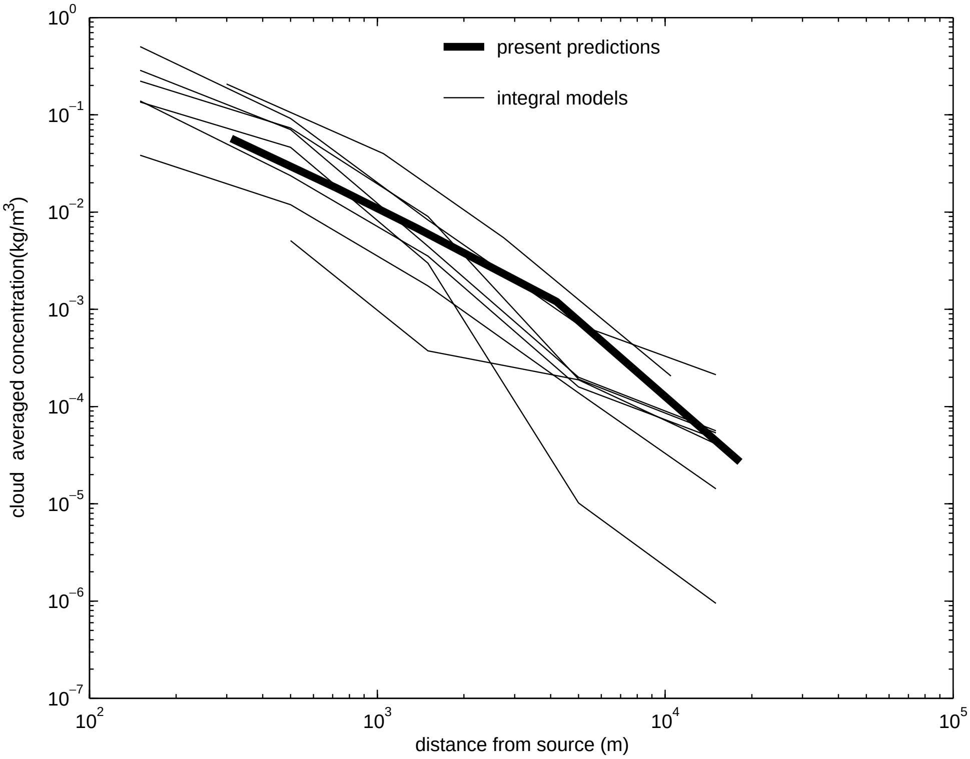

Fig. 3. CAC vs. downwind distance, case P.

As for case A, a large spread of concentrations is evident, especially for larger distances, in line with Mercer's observation that low windspeeds gave rise to a greater range of predictions than high windspeeds.

4.4. *Case T: volume* 2.5×10^5 m^3*, radius 120 m, windspeed 8 m/s*

Fig. 4 shows TWODEE's predictions against downwind distance for case T. Here, TWODEE lies at the lower end of the range but it is nevertheless consistent with those of the integral models' predictions.

4.5. *Cases A–T: overall findings*

Figs. 1–4 show TWODEE predictions are within the range exhibited by the integral models considered by Mercer. The low windspeed cases (A and P) show TWODEE on the upper end of the range, and the high windspeed cases (E and T) show TWODEE near the lower end; although it is not clear whether the tendency is statistically significant.

Interpretation of this is difficult. Each of the integral models had their free parameters optimized to fit the same set of data (Thorney Island). As Mercer pointed out, this was done

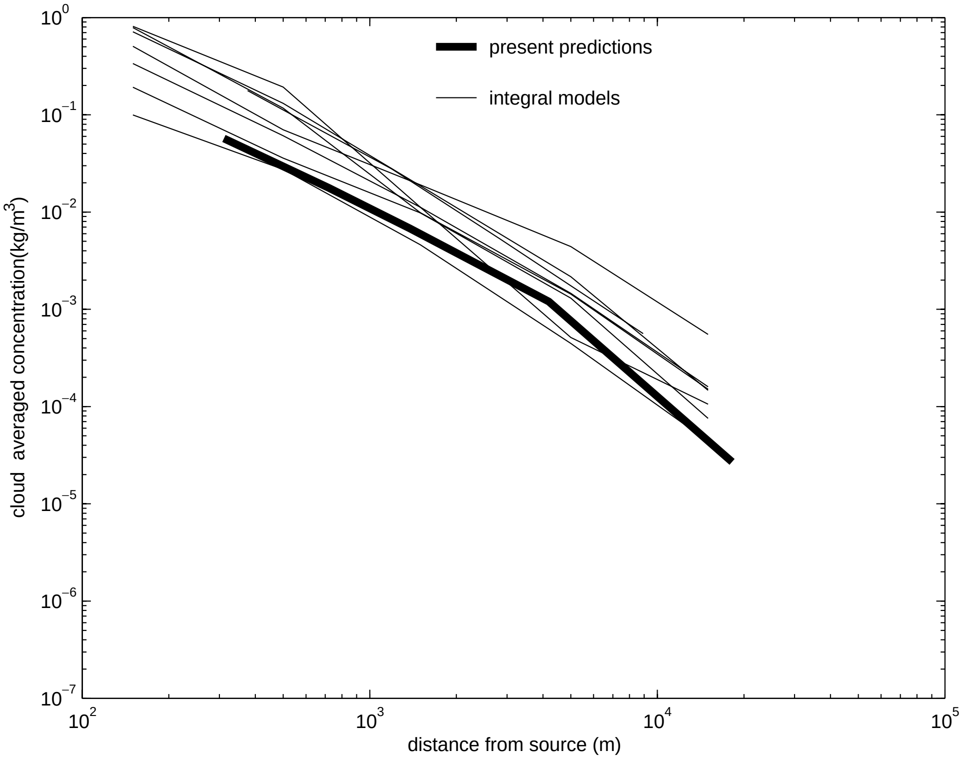

Fig. 4. CAC vs. downwind distance, case T.

in different, non-transparent, ways for each model.[1] One consequence was that objective explanation of why one model's predictions are higher than in another, cannot readily be given: the dataset is complicated, the model is complicated, and here the test cases are complicated.

The approach used in TWODEE was as follows: the parameters chosen were taken directly from Britter [2], or Eidsvik [13]. The parameters used were thus independent of Thorney Island data. TWODEE predictions were then compared with the Thorney Island trials that were included in the Modeller's Data Archive [14] using physical reasoning and goodness of fit measures [14,15]. No compelling evidence emerged to suggest that changing these parameters would give a better model [7,8].

5. Conclusions and discussion

TWODEE has been used to simulate four representative cases of the 25 considered by Mercer [3]. The primary conclusion of this paper is that TWODEE gives predictions that are

[1] A transparent, or literate, methodology is one that is reproducible in the sense that an independent observer would reproduce the exact values of the parameters as the authors [12]. This requires disclosure of the dataset used, the method of optimization, the objective function to be minimized, and the internal coding of the model.

consistent with the integral models considered by Mercer: predicted CACs agree broadly with the consensus.

TWODEE accounts for vertical diffusion but not horizontal diffusion [5]. Overprediction at large distances might therefore be expected, but the model nevertheless agrees with the consensus given by Mercer.

In common with most of the models considered by Mercer, TWODEE did not return useful output for the five cases with a surface roughness of 1.5 m.

One implicit conclusion of this work is that it is *possible* to compare integral model output with shallow layer model output. This is not obvious: integral models use very different assumptions and approaches from shallow layer models. In particular, Mercer [4] found that CAC has no unambiguous definition when (model) concentration profiles are not uniform. Mercer reported that CAC was a strong function of the cloud volume over which averaging took place; and cloud volume is not unambiguously defined when concentration profiles do not fall discontinuously to zero.

Mercer thus found that CAC was not a well-defined concept in many integral models. This work shows that such concerns do not apply to shallow layer models that use objective definitions for cloud height and concentration (Eqs. (1)–(3)): CAC may be defined objectively using Eq. (6), and this appears to agree with the consensus of integral models' predictions.

Integral models typically consider dense gas clouds by analyzing them in terms of a number of regimes; after initial momentum-dominated and buoyancy-dominated phases, a cloud is usually assumed to be passive; some models ensure a smooth transition from one regime to the next.

This multiple-regime approach is not easily transferred to shallow layer models because the whole of the cloud has to be simulated under a single set of model equations. In particular, TWODEE does not account for the horizontal component of diffusion in the passive limit and one consequence of this might be overprediction at large distances. It is not clear that this phenomenon can be modelled in a shallow layer simulation, because shallow layer models have both depth and concentration as variables, and it is difficult to see how both could be diffused in a manner consistent with the passive case but preserving the shallow water solutions of the model in the early buoyancy-dominated regime. The difficulties of such an approach are exacerbated by the fact that some parts of a cloud may be passive and some not; any scheme would have to carry out diffusion in such a way as to approach a Gaussian cross-wind profile on flat ground. There is no obvious method that has all the required properties, although future work may yield a workable solution.

References

[1] C. Nussey, M. Pantony, R. Smallwood, HSE's risk assessment tool, RISKAT, in: Major Hazards: Onshore and Offshore, October 1992, pp. 607–638.
[2] R.E. Britter, Atmospheric dispersion of dense gases, Ann. Rev. Fluid Mech. 21 (1989) 317–344.
[3] A. Mercer, CEA/AEA exchange agreement on external event. Comparison of heavy gas dispersion models for instantaneous releases: final report, Technical Report IR/L/HA/91/6, Health and Safety Laboratory, Sheffield, June 1991.
[4] A. Mercer, et al., Comparison of heavy gas dispersion models for instantaneous releases, J. Hazard. Mater. 36 (1994) 193–208.

[5] R.K.S. Hankin, R.E. Britter, TWODEE: the health and safety laboratory's shallow layer model for dense gas dispersion. Part 1. Mathematical basis and physical assumptions, J. Hazard. Mater. 66 (3) (1999) 211–226.
[6] R.K.S. Hankin, R.E. Britter, TWODEE: the health and safety laboratory's shallow layer model for dense gas dispersion. Part 2. Outline and validation of the computational scheme, J. Hazard. Mater. 66 (3) (1999) 227–237.
[7] R.K.S. Hankin, R.E. Britter, TWODEE: the health and safety laboratory's shallow layer model for dense gas dispersion. Part 3. Experimental validation (Thorney Island), J. Hazard. Mater. 66 (3) (1999) 239–261.
[8] R.K.S. Hankin, Heavy gas dispersion over complex terrain, Ph.D. Thesis, Cambridge University, 1997.
[9] S. Hartwig, Heavy Gas and Risk Assessment—II, Reidel, Dordrecht, 1982.
[10] R.K.S. Hankin, Comparison of the TWODEE model against the Mercer et al. heavy gas dispersion code comparison exercise, Technical Report RAS/96/19, Health and Safety Laboratory, Sheffield, 1996.
[11] H.A. Panofsky, J.A. Dutton, Atmospheric Turbulence: Models and Methods for Engineering Applications, Wiley, New York, 1984.
[12] A.J. Rossini, Literate statistical practice, in: K. Hornik, F. Leisch (Eds.), Proceedings of the Second International Workshop on Distributed Statistical Computing, Technische Universität Wien, Vienna, Austria, March 2001.
[13] K.J. Eidsvik, Dispersion of heavy gas clouds in the atmosphere, Technical Report NR 32/78; 25077, Norwegian Institute for Air Research, Lillestrøm, Norway, 1978.
[14] S.R. Hanna, J.C. Chang, D.G. Strimaitis, Hazardous gas model evaluation with field observations, Atmos. Environ. A 27 (15) (1993) 2265–2285.
[15] S.R. Hanna, D.G. Strimaitis, J.C. Chang, Hazard response modeling uncertainty (a quantitative method), vol. 1, User's guide to software for evaluating hazardous gas dispersion models, Technical Report F08653-89-C-0136, Sigma Research Corporation, Westford, MA, USA, September 1991.