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TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion Part 3: Experimental validation (Thorney Island)

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Abstract

Part 1 of this three-part paper described the mathematical and physical basis of TWODEE, the Health and Safety Laboratory's shallow layer model for heavy dispersion. In part 2, the numerical solution method used to simulate the TWODEE mathematical model was developed; the flux correction scheme of Zalesak [S.T. Zalesak, Fully multidimensional flux-corrected transport algorithms for fluids, Journal of Computational Physics, 31 (1979) 335–362.] was used in TWODEE. This paper compares results of the TWODEE model to the experimental results taken at Thorney Island [J. McQuaid, B. Roebuck, The dispersion of heavier-than-air gas from a fenced enclosure. Final report to the U.S. Coast Guard on contract with the Health and Safety Executive. Technical Report RPG 1185, Safety Engineering Laboratory, Research and Laboratory Services Division, Broad Lane, Sheffield S3 7HQ, UK, 1985.]. There is no evidence to suggest that TWODEE predictions could be improved by changing any of the entrainment parameters from generally accepted values [R.K.S. Hankin, Heavy gas dispersion over complex terrain, PhD thesis, Cambridge University, 1997.]. The TWODEE model was broadly insensitive to the exact values of the entrainment parameters. Crown Copyright © 1999 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

The mathematical basis of the TWODEE model was introduced in part 1 of this three-part paper. Part 2 of this paper validated the computational scheme by comparing TWODEE output with theoretical results.

For credibility in land use planning, it is necessary to compare TWODEE predictions with experimental data taken from large-scale outdoor releases. This comparison will allow some account to be made of the suitability of the model entrainment terms (which are essentially free parameters) as well as the overall model structure.

2. Model quality and model evaluation

The determination of the best free parameters to use in the present model should be part of the wider activity of model quality improvement. The quality of heavy gas dispersion models is discussed by Britter [1], who considers features of models such as computational expense and ease of use in addition to physical accuracy. Here, attention will be confined to scientific assessment, and this will be achieved by analyzing the discrepancies between prediction and experiment.

2.1. Goodness-of-fit measures (GFMs)

Large scale heavy gas dispersion experiments typically generate a large amount of data, as reported by McQuaid and Roebuck [2]. This means that direct comparison of predicted concentrations to measured concentrations is not straightforward.

Choosing a small number of concentration time traces for detailed comparison with model predictions as a sole method of model assessment is unacceptable for two reasons. Firstly, this is sensitive to the (subjective) choice of traces to be used; and secondly, such comparison yields little, if any, information about systematic model errors.

It is therefore necessary to define objective measures of how closely experimental results are predicted by a model; the term 'GFM' will be used to cover all such quantities. In addition to meeting the comments above, the definition of a GFM elucidates precisely what features of the experimental results the model is attempting to reproduce. In general, GFMs are interpreted as the 'distance' of the model predictions from the data; thus a smaller GFM indicates a better fit. Different GFMs highlight different aspects of a model's predictions.

It is the case that a small GFM can obscure serious shortcomings in a model. This may be mitigated by the use of a large number of GFMs and optimizing with respect to some overall quantity, but even this approach has disadvantages that are discussed below. Physical interpretation of a model's results must also be made, even though such considerations cannot be objective.

Wheatley et al. [3] considered the use of GFMs to determine the top entrainment parameter α_T in a model they were developing, and it was observed that

> It is tempting to think that a GFM could be defined for the trials as a whole and a single overall optimum value found for α_T ... This approach would, however, be misleading for a number of reasons. Firstly, if an overall value of α_T is defined, then differences that occur between the [model] fit and data are not entirely random; there is also a systematic component, according to the choice made for the entrainment model. Secondly, the accuracy to within which the optimum value of α_T for a given trial is determined is not commensurate with the minimum size of the GFM;... this could lead to unjustified biasing in favour of a few trials merely because they show less scatter.

Wheatley et al. went on to determine a value of α_T for each of the Thorney Island instantaneous releases. This work will essentially follow Wheatley et al. by considering TWODEE predictions of a single Thorney Island trial, and then using the model for the remaining trials.

2.1.1. The GFMs of Hanna et al. [4]

Following earlier work on the evaluation of air quality models [5,6], Hanna et al. considered heavy gas dispersion [4] and defined the geometric mean bias MG, the geometric variance VG, and the correlation coefficient R as follows:

$$\mathrm{MG} = \exp\left[\overline{\ln(C_o/C_p)}\right] \tag{1}$$

$$\mathrm{VG} = \exp\left[\overline{\ln(C_o/C_p)^2}\right] \tag{2}$$

$$R = \overline{(\ln C_o - \overline{\ln C_o})(\ln C_p - \overline{\ln C_p})}/(\sigma_{\ln C_p} \cdot \sigma_{\ln C_o}) \tag{3}$$

where C_o and C_p are the observed and predicted peak concentrations, and an overbar indicates an average over one particular group of concentration measurements. A perfect model has MG = VG = R = 1. In addition, FAC2 was defined to be the fraction of C_p that were within a factor of 2 of C_o.

This set of GFMs implicitly uses the lognormal distribution of concentration and will be used throughout the remainder of this paper. Hanna et al. set C_p to sensor noise level if $C_p = 0$ and this device will be used here.

Hanna et al. calculated the three GFMs above for a number of datasets and took a weighted mean of these to be representative of the model as a whole. They were thus able to assess the goodness-of-fit of 14 heavy gas dispersion models to the 'Goldfish' experiments [7] and models were represented on a plane as points, the x- and y-coordinates being the MG and the VG score of that model. Models with small MG and VG scores were thus represented as points close to the origin.

2.1.2. Stochastic uncertainty and GFMs

Britter [1] points out that VG is bounded below by stochastic uncertainty and data errors and notes that

> ...even if the model physics error was zero there is an underlying or inherent uncertainty due to the stochastic nature of the problem and to data errors

Davies [8], commenting on Hanna et al. [4], presents statistical arguments to support Britter's statements. Here, attention will be confined to assessment of the present model's physical accuracy and its ability to predict experimental data.

3. Experimental data for evaluation of GFMs: the modellers' data archive (MDA)

Large scale heavy gas dispersion experiments, all of which took place on level or near-level ground, have been summarized by Hanna et al. [4] in the MDA. The MDA was originally created in order to compare the results of a number of dispersion models with experiment. This was done by placing the results of a number of dispersion trials in a common format; the format included sufficient information to run the dispersion models, and a condensed subset of the experimental results.

A brief description of nine dispersion trials was given by Hanna et al. [4]. Two of these were passive experiments and six measured the dispersion of substances whose behaviour was strongly influenced by thermodynamic effects such as phase changes and thus not considered here. This leaves two experiments: the instantaneous and continuous Thorney Island trials [2], and use will be made of those Thorney Island trials that appear in the MDA.

3.1. Repeat- and atmospheric-variability

Each Thorney Island release was performed only once: results are therefore one realisation from an ensemble. Puttock and Colenbrander considered ensemble statistics in the context of risk assessment [9] and concluded that a useful model of heavy gas dispersion should produce a typical member of the ensemble as output (and not ensemble averaged values). Carn et al. [10], discussing variability, observed that prior agreement on criteria for typicality should be adopted; and Chatwin [11] emphasized the importance of clear definition of the underlying ensemble. Carn et al., commenting on Puttock and Colenbrander's work, stressed that judicious choice of ensemble would reduce the discrepancies between useful model predictions and ensemble average traces discussed by Puttock and Colenbrander. The comments of Carn et al. [10] are partially accounted for in this work by using a large number of datapoints from the Thorney Island releases.

Hall et al. [12] has investigated the repeat variability of instantaneously released heavy gas clouds. He used a scale model of the release mechanism used at Thorney Island [2] and carried out either 50 or 100 repeats. Hall reported that

> the ratio of the 10th to the 90th percentile is typically of order 2, with occasional larger excursions which do not exceed an order of magnitude...this is the component of the variability due to a combination of variations in the self-driven flow within the gas cloud and of small scale atmospheric turbulence of the sort reproduced in wind tunnel models.

Hall went on to discuss the additional variability occurring in practical situations as a result of larger-scale turbulent fluctuations not reproduced in wind tunnels.

Wilson [13], considering concentration fluctuations in hazard assessment, states that "The peak concentration observed during any one [dense gas] release event can vary by a factor of 10 among the members of an ensemble of identical releases into the same atmospheric conditions." This greater variability was due to atmospheric phenomena—such as wind direction swings—that are not reproduced in wind tunnels. Wilson stated that dense releases would meander as they entrain air with crosswind velocity fluctuations.

Thus agreement with Thorney Island data to within a factor of about 3 is the best that could reasonably be expected. Variability is one reason why comparison of a large number of datapoints is required, as then underlying systematic trends may be distinguished through the scatter.

4. Model validation: Thorney Island

TWODEE will now be evaluated by comparing its predictions with field data from the Thorney Island experiments [2]. The main form of analysis is the comparison of peak concentrations. The evaluation method used will be the investigation of systematic mispredictions (trends); any such trends would be indicative of problems either in the physical assumptions made in the model, or the choice of free parameters. Additional benefits from this analysis will include estimating the likely errors made by the model, and the sensitivity of the model to the variation of the free parameters.

4.1. Overview of methodology

Given that no overall 'best' model may be found (Wheatley et al.'s [3] comments reproduced on page 3 discusses this) it is neither possible nor desirable to 'optimize' the constants in the present model to the Thorney Island dataset. The general approach will be as follows.

(1) A reasonable set of constants will be chosen for the model; see part 2 of the present paper. These constants will either be generally accepted values, or values taken from other heavy gas dispersion models. The parameters thus obtained are independent of the Thorney Island experiments as they were determined before 1982.

(2) For certain of the Thorney Island Instantaneous Trials (restricted to those included in the MDA), the model will be run with the same source and meteorology. The results will be compared using both GFMs and physical reasoning.

(3) The constants used will be altered if necessary to obtain better agreement.

The comparison method chosen uses all sensors detecting gas. This gives an objective comparison: there is no (subjective) choice of which sensor data to use. Although Thorney Island data has been used for model comparison before, by Hanna et al. [4], that comparison used only centreline concentrations. The present model is being used here to predict peak concentrations in three dimensional space, so higher MG- and VG-scores might be expected.

Peak concentration will be used as the primary comparison statistic, being of industrial interest and physical meaning. However, peak concentration depends on the averaging time used and this is discussed below.

4.2. Peak concentration and averaging time

Nussey et al. [14] consider measured peak concentration as a function of time averaging period used. They concluded that "0.6 s represents an averaging time that is reasonably consistent with the criterion that [instrument] noise should be suppressed."

Peak concentrations calculated on a 0.6 s (moving-point) averaging time basis have been used here, following Hanna et al. [4].

This system filters out high-frequency fluctuations which are not simulated with the present shallow layer model, which cannot resolve phenomena on timescales $\leq (h/g')^{1/2}$. A 0.6 s averaging time is thus appropriate for any model not simulating the fine-scale structure of the cloud, as here.

The present model describes a spreading heavy gas cloud as a function of ground position and time; it is thus possible to compare very much more than peak concentrations against downwind distance. This study will therefore consider the response of every sensor that detects gas, using the full three-dimensional coordinates of the point (downwind distance, crosswind distance, and altitude). This will allow investigation of such aspects of the cloud as its width, and height.

The ratio of observed to predicted concentrations may be plotted as functions of downwind distance, crosswind distance, or sensor altitude. Examination of these residual plots would show any systematic error that would indicate incorrect entrainment parameters.

4.3. Ensemble variation and model predictions

The present model does not include the random effects of turbulence: it is deterministic. Model predictions are therefore interpreted as representative measures of the relevant ensemble. The method of comparison used compares large numbers of peak concentrations in one realisation to the predictions of the present model on a logarithmic scale.

As discussed above, peak concentrations in an ensemble of Thorney-type releases have a range of about an order of magnitude. This variability is one reason why large numbers of peak concentrations are compared: any trends that are coherent over an experiment can reasonably be attributed to physical causes (and not random variation).

4.4. Code comparison: selection of appropriate Trials

The Thorney Island Phase One instantaneous release experiments comprised 16 releases [2]. Of the 16 releases, seven are not suitable for use here: one was a test run, the release mechanism failed for one, the wind changed in two, and air contaminated the gas bag to an unknown extent in three. The nine remaining Trials constitute the MDA.

For the purposes outlined above, a detailed discussion of three experiments will be made; the experiments chosen were numbers 08, 09, and 13. These Trials were chosen as they spanned the full range of windspeeds (Trial 09 had the slowest windspeed and Trial 13 the fastest); Trial 08 was included as it had the greatest number of useful sensor records. Each of the nine Trials included in the MDA was matched against the present model by the present author [15]; the Trials chosen here were not exceptional in terms of GFMs in any way, although each Trial was different.

5. Thorney Trial 08

Thorney Island Trial 08 was a particularly successful one: a large proportion of the sensors operated satisfactorily, and the wind direction almost bisected the sensor array; for this reason more analysis has been carried out on this Trial than the others. In particular, the present model has been tested with different entrainment parameters against the experimental results from this Trial. Several methods of analysis will be presented.

- The vertical concentration profile to be used will be investigated. Three different assumed vertical concentration profiles (exponential, Gaussian, and uniform) will be used and their results compared.
- Differing values of the entrainment parameters will be used and the results compared with experiment. The ‘base case’ used takes values from theoretical studies and previous heavy gas dispersion models. It is shown that there is no basis for using entrainment parameters that differ from these default values.
- Residual analyses are presented and where severe over- or under-prediction occurs, a physical explanation is sought (for example, many under-predictions are due to the sensor in question lying outside the predicted plume path).

5.1. Vertical concentration profiles

One of the aims of this analysis was to investigate the suitability of different vertical concentration profiles. Hankin [16] shows how vertical concentration profiles may be represented in a shallow layer model; the equation of state may be used to link the concentration to the density ρ. Hankin shows that

$$\rho(z) = \rho_a + (\bar{\rho} - \rho_a)\frac{4}{\pi S_1}\exp\left[-\left(\frac{2z}{S_1 h\sqrt{\pi}}\right)^2\right] \text{ Gaussian distribution,} \tag{4a}$$

$$\rho(z) = \rho_a + (\bar{\rho} - \rho_a)\frac{2}{S_1}\exp\left[-\frac{2z}{h}\right] \text{ Exponential distribution,} \tag{4b}$$

$$\rho(z) = \rho_a + (\bar{\rho} - \rho_a)\frac{1}{S_1}H[z-h] \text{ Uniform distribution.} \tag{4c}$$

where H is the Heaviside operator with $H(x) = 0$ if $x < 0$ and unity otherwise; S_1 is the dimensionless shape parameter defined in part 1 of the present paper, and $\bar{\rho}$ is the depth averaged density.

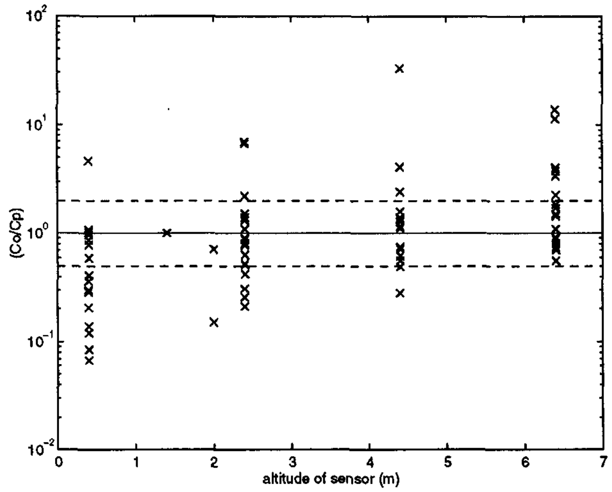

Fig. 1. Thorney Island Trial 08: C_0 / C_p as a function of the altitude of the sensor. Exponential vertical concentration distribution.

The approach used here is to use each of the three distributions described in Eqs. (4a), (4b) and (4c) and assess the performance of the model under each one. Hankin [16] considers a wider range of vertical profiles but shows that there is no reason to use more complex forms.

Vertical profiles may be assessed by plotting the residuals C_0/C_p for each sensor as function of altitude. Figs. 1–3 show the residual analysis for Thorney Trial 08 using exponential, Gaussian, and uniform vertical profiles, respectively. These graphs show that there is a slight tendency to over-prediction (see Table 1 for a precise statement)

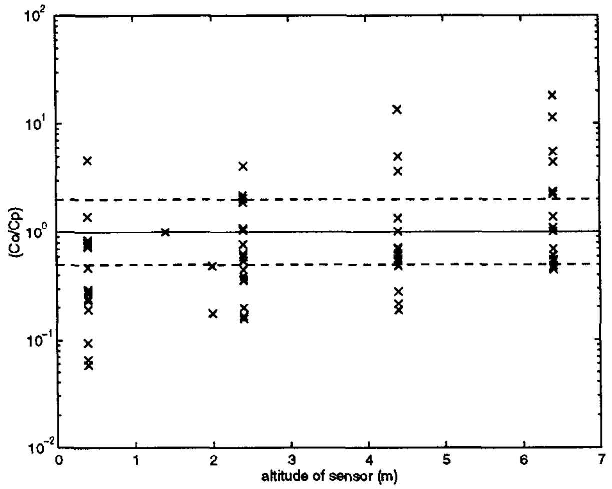

Fig. 2. Thorney Island Trial 08: C_0 / C_p as a function of the altitude of the sensor. Gaussian vertical concentration distribution.

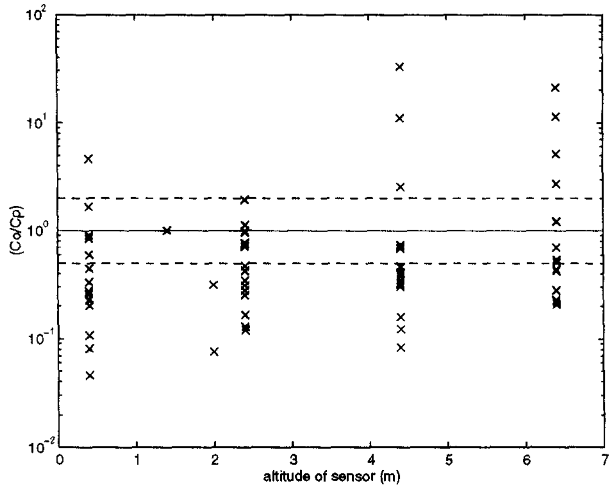

Fig. 3. Thorney Island Trial 08: C_0 / C_p as a function of the altitude of the sensor. Uniform vertical concentration distribution.

and a slight systematic trend for the lowest sensors to be over-predicted and the highest sensors to be under-predicted. These trends are, however, not statistically significant.

Table 1 shows the four GFM scores defined by Hanna et al. calculated using the 73 sensors detecting gas at Trial 08, for each of the three vertical profiles. It is clear that the exponential fit is the best, followed by Gaussian, and the top hat is the worst. Exponential concentration distributions will therefore be used for this report, although different distributions may be considered if a residual analysis against sensor altitude shows any trend.

An exponential vertical concentration distribution appears to be the most appropriate. Only this distribution will be used for the remaining Trials, but a significant systematic trend for over- (or under-) prediction with increasing altitude might suggest that another distribution would fit the data better.

5.2. Variation of TWODEE entrainment parameters: $u_{ent} = au_* / (1 + bRi)$

As discussed in Section 4.1, the base case model uses entrainment parameters that are set to standard values obtained from the literature. Here, the effect of changing them is investigated.

Table 1
GFMs for three vertical concentration distributions; Thorney Island Trial 08

Distribution	GFM (rank)			
	MG	VG	R	FAC2
Exponential	0.80 (1)	3.85 (1)	0.52 (2)	0.52 (1)
Top hat	0.51 (3)	7.10 (3)	0.49 (3)	0.30 (3)
Gaussian	0.70 (2)	4.10 (2)	0.53 (1)	0.41 (2)

Bracketed figures show rank—1, 2, and 3 for first, second, or third, respectively.

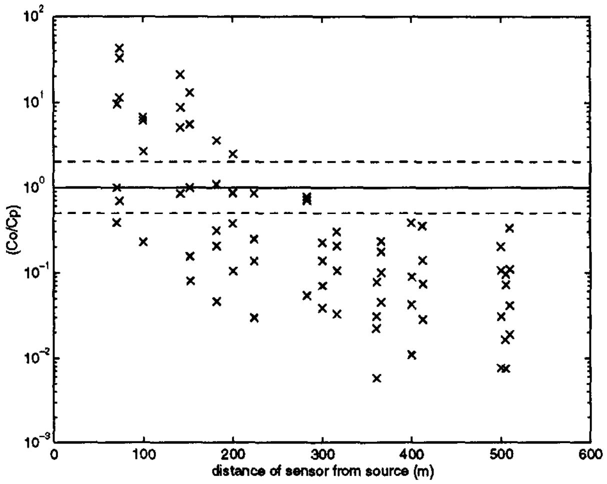

Fig. 4. Thorney Island Trial 08: C_o / C_p as a function of the distance of the sensor from the source. Model using $a = 0.1$.

Top entrainment terms are usually of the form $u_{ent} = au_* / \{1 + b\mathrm{Ri}\}$, where $a = 0.4$ and $b = 0.125$ are common choices. These values for a and b were used as a 'base case'. The existence of any significant trends would then used as case for alteration of either a or b.

Figs. 4–6 show C_o/C_p as a function of distance with a equal to 0.1, 0.4 (von Karman's constant), and 0.7. The purpose of this exercise was two-fold: first to ascertain the sensitivity of the model to a, and second to determine whether the experimental data

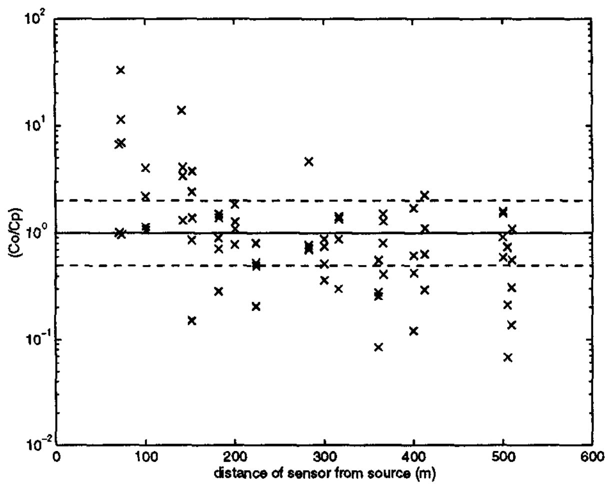

Fig. 5. Thorney Island Trial 08: C_o / C_p as a function of the distance of the sensor from the source. Model using $a = 0.4$.

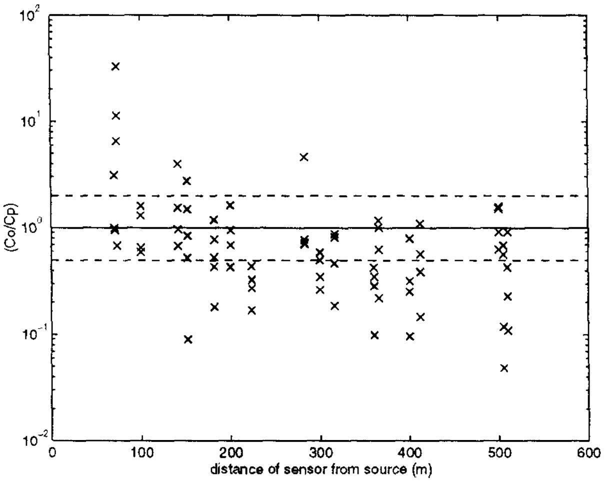

Fig. 6. Thorney Island Trial 08: C_o / C_p as a function of the distance of the sensor from the source. Model using $a = 0.7$.

warrant a value for a other than the preferred and theoretically supportable value of 0.4. This method of analysis also allows some estimation of the errors likely to be made when using the present model to estimate peak concentration as a function of position.

As the value of a increases, more entrainment occurs through the cloud top, with consequent faster dilution (both in space and time; the windspeed is held constant). For large values of a, therefore, it would be expected for large distances to be under-predicted compared to small distances; the opposite effect should be evident for small values of a. This exercise will not result in a 'best' value for a; the purpose is to assess whether there are grounds for changing the parameters used.

Figs. 4–6, taken together, are more similar to one another than might be expected; each exhibits about the same magnitude of scatter; and each has severe under-predictions at small distances (the behaviour of the model close to the source is further discussed below); and each exhibits a tendency to over-prediction for distances larger than $\simeq$ 100 m. Only Fig. 4 ($a = 0.1$) exhibits a systematic trend: over-prediction tends to increase with distance, as might be expected for such a small value of a.

Each of Figs. 4–6 exhibit large scatter. This could be due to several factors, discussed on page 5. If residual analyses are presented for all meaningful variables and no trends found, then the remaining 'unexplained' mispredictions may be interpreted as manifestations of the random nature of the turbulent dispersion occurring at Thorney Island, together with random noise imposed on the sensor records.

The uniformity of scatter between Figs. 4–6 shows that the model is not very sensitive to the value of a. This is encouraging from a pragmatic viewpoint because the model does not appear to depend on the exact value used for a, and indeed Hankin [16] shows that the model performance is not significantly affected by changing a within the range 0.2–0.7. (Fig. 7)

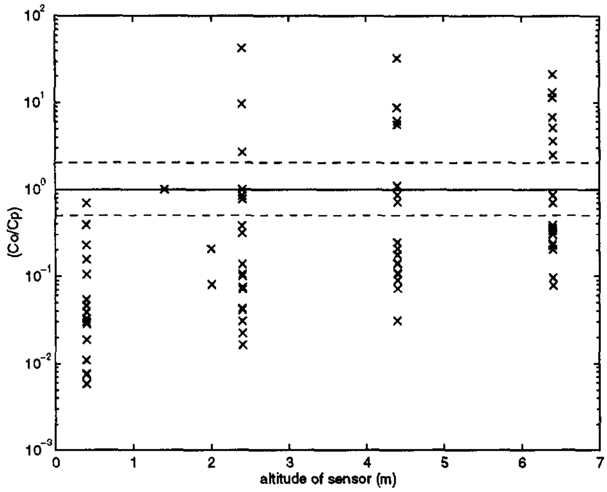

Fig. 7. Thorney Island Trial 08: C_o / C_p as a function of the altitude of the sensor. Model using $a = 0.1$.

It is possible to alter the parameter b, although one might expect the model to depend more weakly on b than on a. Hankin [16] showed that there was no reason to use anything other than the standard value of 0.125 for b.

5.3. Results of varying a and b: conclusions

The values for a and b suggested by Britter [17] and Rosenzweig [18] will be used for simulating the remaining Trials, because other values did not perform better against experiment. However, this work is not conclusive: if any significant trend is found, one of the investigative tools available is to change these entrainment parameters and analyse the results. (Fig. 8)

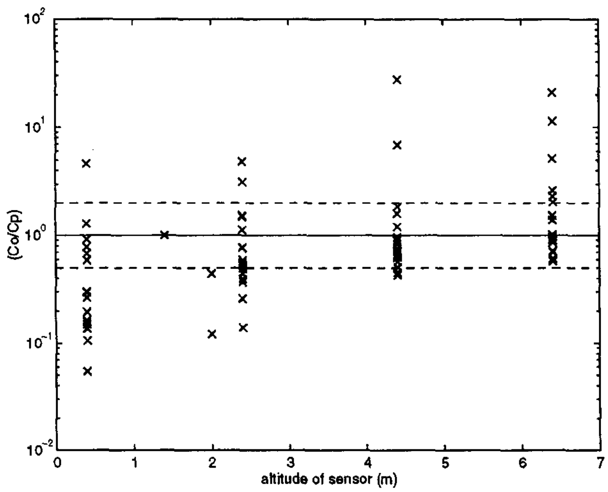

Fig. 8. Thorney Island Trial 08: C_o / C_p as a function of the altitude of the sensor. Model using $a = 0.7$.

5.4. The model using the default values for a and b

The possibility that the mispredictions above are systematically linked to crosswind distance or sensor altitude is now investigated using the default values of a and b. Residual analyses for C_0/C_p as functions of distance from source, crosswind distance and sensor altitude are presented. However, a discussion of the predicted cloud footprint is presented first to place the more formal analysis in context.

Fig. 9 shows a plan view of the site. Each sensor detecting gas is seen as a circle, the source is the small square at (400, 200), and the irregular lines are the contours of predicted dose.

With the exception of the sensor mast at (200, 400), only sensors detecting gas were predicted to do so. This is evidence that the cloud width is correctly modelled, although this should be interpreted together with the residual analysis.

5.4.1. Residual crosswind analysis for the default case

Fig. 10 shows the crosswind residual analysis for Thorney Trial 08. No trend is visible, although three extreme under-predictions may be seen at a crosswind distance of about +75 m (they are the sensors at (450, 250) and are discussed by Hankin [16]).

The lack of systematic crosswind dependence of C_0/C_p is further evidence that the plume width is correctly modelled: if (for example) the predicted plume were too narrow, points at high absolute crosswind distance would be under-predicted and the residual analysis graph would be a U shape.

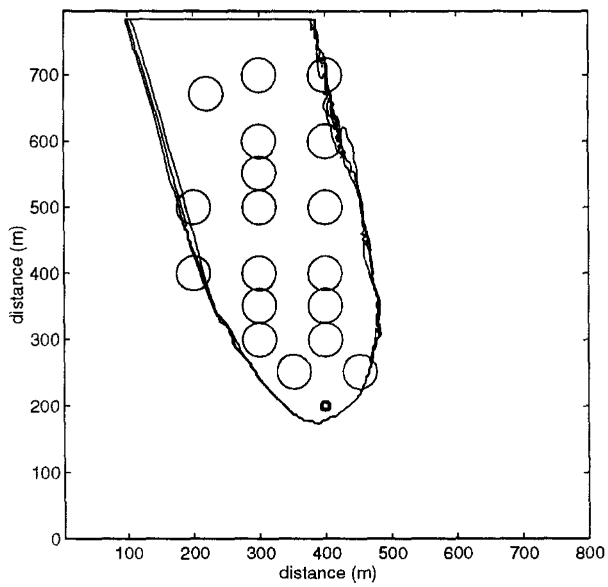

Fig. 9. Thorney Island Trial 08: contours of predicted dose (irregular lines; values 10^4, 10^5, and 10^6 ppm^2 min) and sensors detecting gas (circles). Small square at (400, 200) is the source.

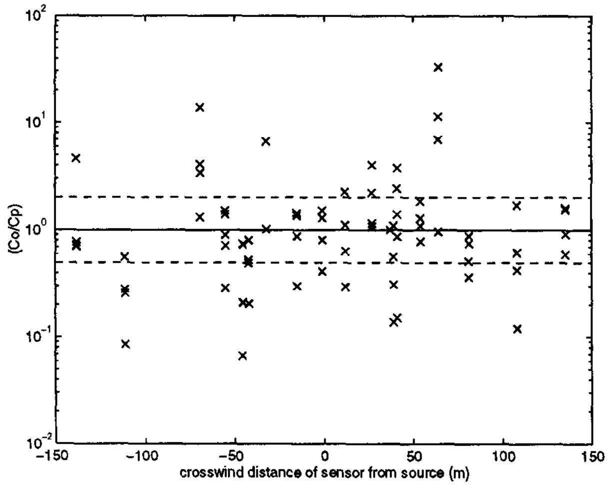

Fig. 10. Thorney Island Trial 08: C_o / C_p as a function of crosswind distance.

5.5. *Individual sensor records*

The residual plots presented include some severe over- and under-predictions. These outliers (only two sensors positions were over-predicted by more than a factor of 10) are discussed by Hankin [16]. Many of the under-predictions are caused by the predicted plume lying outside the sensor mast in question and are thus largely independent of the entrainment parameters used; but the over-predictions require a different analysis. It was found that many of the over-predictions are intimately connected with the vertical concentration profile that is fitted to the model at the post-processing stage; thus any sensor record should be viewed in the context of the other sensors on the same mast.

Fig. 11 shows the predicted and observed concentration traces at (450, 250, 0.4).

5.6. *Conclusions from Trial 08*

In this section, Thorney Island Trial 08 has been simulated with the present model. This Trial, being particularly successful, contains more analysis than the other Trial comparisons.

There was no evidence to suggest that changing the default entrainment parameters used in the model would give better agreement with experimentally determined peak concentrations. Since there is a body of theoretical and other evidence supporting the use of this choice of entrainment parameters, these will be used. However, if any other Trials display any systematic trend, then one analytical tool available would be to vary the default parameters.

One of the outcomes of varying a and b was to show that the model is relatively insensitive to the exact values used. This is encouraging as it suggests that precise determination of a and b is unnecessary for risk assessment purposes.

Using the default values of a and b, three vertical concentration profiles were examined. The model predictions remained largely insensitive to changing the assumed profile, but an exponential profile gave the best agreement with experiment.

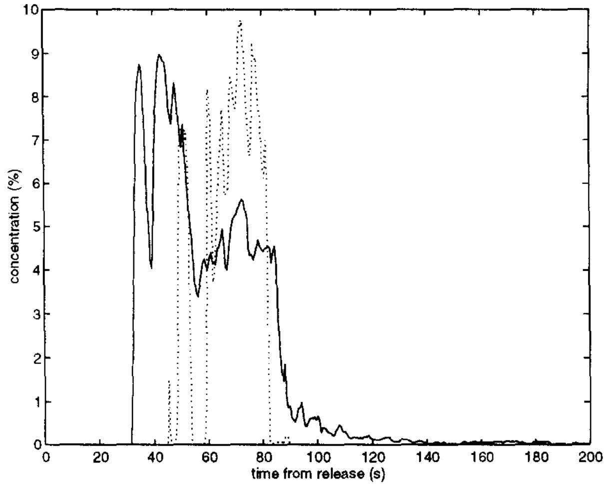

Fig. 11. Thorney Island Trial 08: predicted (...) and experimental (—) Eulerian concentration traces at (450, 250, 0.4). Model using a 1 m grid size.

The work in this section suggests that, for the remaining Trials considered, the following protocol is appropriate:

- the three residual plots (C_0/C_p as a function of distance from source, altitude, and crosswind distance) are produced;
- any trends found investigated from a physical viewpoint including change of the entrainment parameters a and b;
- any outlying points further investigated and any physical explanation for the misprediction given.

6. Thorney Trial 09

Thorney Trial number 09 was conducted at the lowest windspeed of all the Phase 1 Trials (1.7 m/s). A total of 56 sensors detected gas; the mean wind direction was 26.9° to the right of the sensor array centreline.

Fig. 12 shows the positions of the sensors detecting gas and the outline of the predicted plume as determined by the dose experienced at ground level. It is clear that a number of sensors that detected gas in the experiment are outside the plume as predicted by the present model. [2] That the predicted plume does not include these sensors is clearly due to the modelling of the earliest phases of the release, during which the upwind spread of the cloud is determined (at no other time does the cloud have enough potential energy to travel against the wind).

[2] The predicted gas concentration is defined in these circumstances to be the noise level of the sensors. That the model correctly predicted *absence* of gas for the remaining sensors with the exception of the sensor at (400, 500) is encouraging.

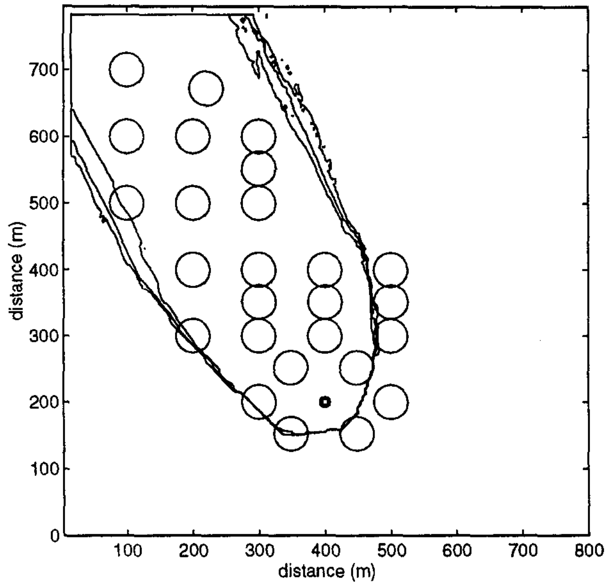

Fig. 12. Thorney Island Trial 09: contours of predicted dose (irregular lines; values 10^4, 10^5, and 10^6 ppm^2 min) and sensors detecting gas (circles). Small square at (400, 200) is the source.

Nine sensors that were deemed to have detected gas had predicted peak concentrations of zero—or sensor noise level. However, peak concentration data should be interpreted in context. The five ground positions of these sensors are visible as the rightmost four sensors in Fig. 12 with an extra location at (450, 150). Although in each case, the peak concentration is well above the nominal sensitivity, each trace reveals that

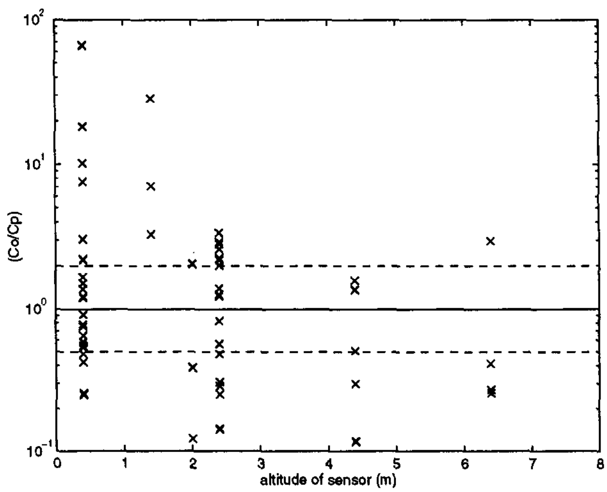

Fig. 13. Thorney Island Trial 09: C_o / C_p as a function of the altitude of the sensor.

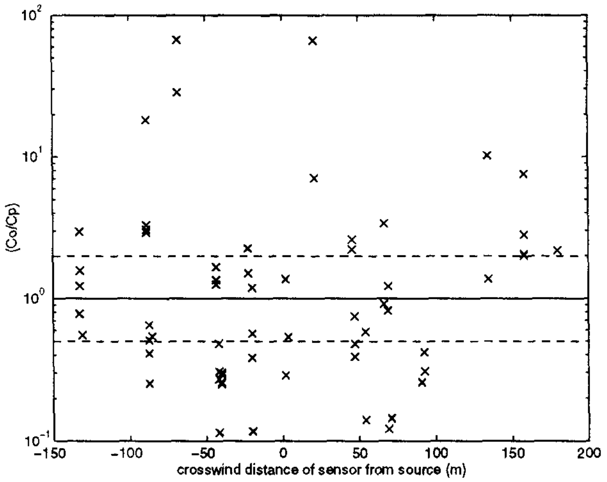

Fig. 14. Thorney Island Trial 09: C_o / C_p as a function of crosswind distance.

the upper sensor detected gas but only transiently (the timescale for judging transience is $\sqrt{h/g'} \sim 1$ s). It is reasonable to say that the cloud is $\gtrsim 1.4$ m high in this region; such formations are poorly handled by the present model, as discussed by Hankin [16].

Figs. 13 and 14 show C_o/C_p vs. altitude and crosswind distance, respectively. No systematic trends are seen, except for a cluster of under-predictions at small altitudes in Fig. 13. This is discussed with reference to distance from source below.

Fig. 15 shows the residuals plotted against distance from source. This graph shows no distinct trends (apart from the near sensors to be under-predicted because they are outside the predicted plume), again indicating that the model with default entrainment

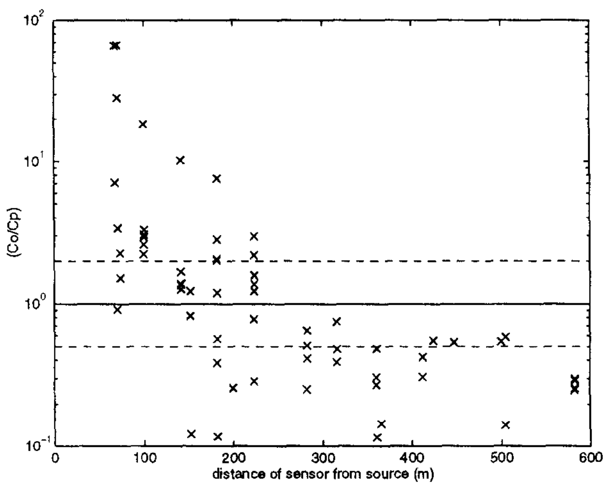

Fig. 15. Thorney Island Trial 09: C_o / C_p as a function of distance from source.

parameters gives no systematic trends. The general under-prediction at small distances seen in Fig. 15 is due to the five sensor positions which experienced gas but were not inside the predicted plume.

7. Thorney Trial 13

Thorney Trial number 13 was conducted at the highest windspeed of the programme, 7.1 m/s at the reference height of 10 m. Although some buffeting of the gas bag was observed at this high windspeed, the release was judged to be successful.

Fig. 16 shows the path of the predicted plume, together with the locations of the sensors that detected gas. It is evident that the sensor at (500, 600), while detecting gas, is outside the predicted plume, leading to an over-prediction factor of ~ 7. As no sensors to the right of those shown were deployed at the site, it is reasonable to hypothesize that the plume width is being simulated approximately correctly, but at an incorrect bearing. The wind direction used in the present simulation was taken directly from databook 19 [19].

Evidence for the hypothesis that an inappropriate wind direction was used is provided by Fig. 17, in which the C_0/C_p values alternate between over- and under-prediction from about 300 m from the source. This is due to the coincidence that the sensors at successively larger distances from the source alternate between under-prediction (lying

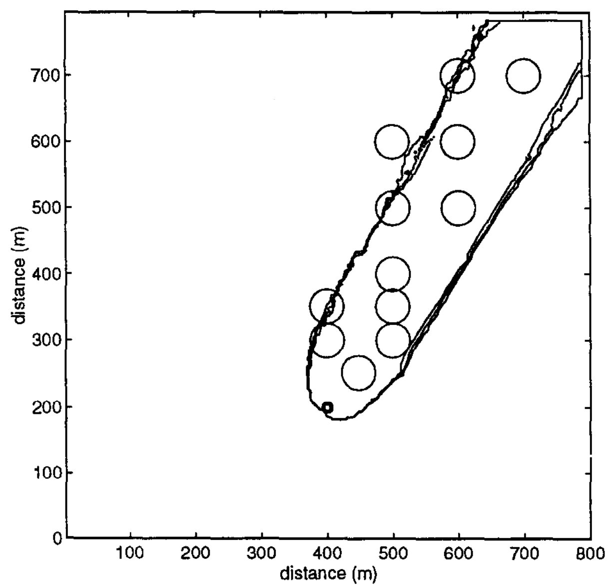

Fig. 16. Thorney Island Trial 13: contours of predicted dose (irregular lines; values 10^4, 10^5, and 10^6 ppm^2 min) and sensors detecting gas (circles). Small square at (400, 200) is the source.

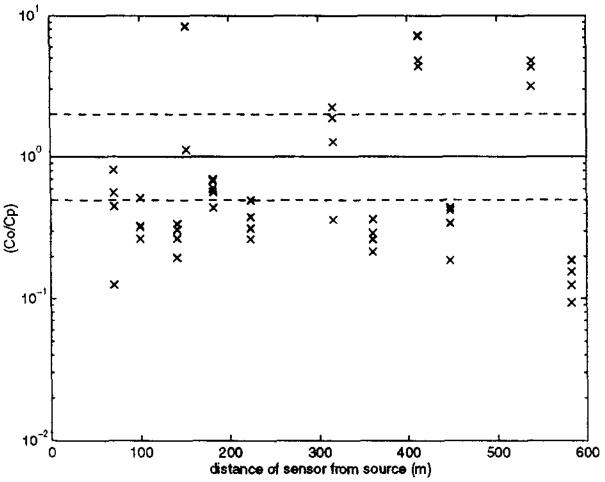

Fig. 17. Thorney Island Trial 13: C_o / C_p as a function of distance from source.

outside the predicted plume but inside the experimental plume) and over-prediction (lying close to the centre of the predicted plume but at the edge of the experimental plume). Successive points alternate between being closer to the predicted plume centreline than the real plume centreline, and being further away.

Figs. 17–19 show the standard residual analyses of C_o/C_p against distance, altitude, and crosswind distance, respectively. Only Fig. 19 shows a trend; the sensors at the most negative crosswind distances were under-predicted as the simulated plume did not pass over them.

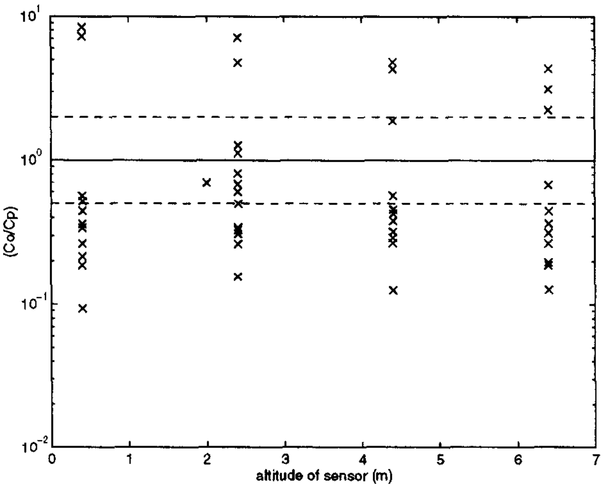

Fig. 18. Thorney Island Trial 13: C_o / C_p as a function of the altitude of the sensor.

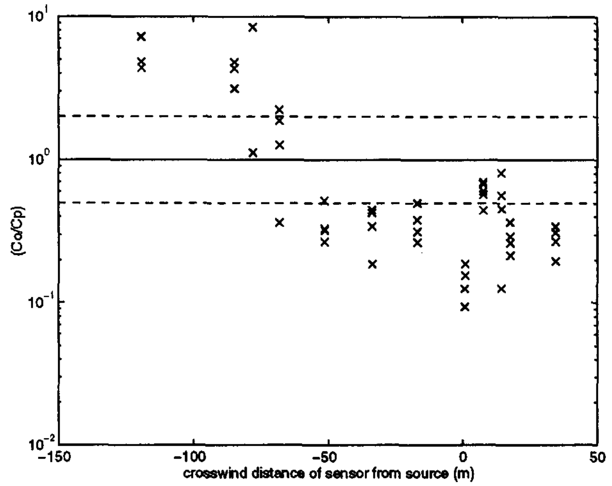

Fig. 19. Thorney Island Trial 13: C_o / C_p as a function of crosswind distance.

It is logical to investigate the nature of the experimental concentration trace at the leftmost gas detector seeing gas (the gas signal could have been transient or registered only at one height). There was gas at (500, 600) and that the signal was not limited to the lowest sensor [16]. It is also the case that the peak concentration at this level was almost independent of height for the sensors at this mast.

In light of these observations it is reasonable to conclude that the wind bearing of 30.8° given in the databook is not an absolute figure and should be viewed in the context of both the experimental concentration traces and the environmental history at the site; TWODEE uses a uniform steady ambient velocity field. [3]

The appropriateness of the given wind bearing may be tested by running the present model with a different wind direction, and results are presented below.

8. Thorney Trial 13: wind direction change

As discussed above, the sensor records at Trial 13 are to some extent inconsistent with the reported wind direction. In this section, the present model will be used to simulate Trial 13, but with a different wind direction.

Fig. 20 shows a plan view of the site. The cloud path, as illustrated by time-integrated dose contours, may be seen to be at an angle of 25° from the array centreline; this more

[3] The 30.8° was obtained at location (400, 50) at 10 m altitude. The trace from this instrument exhibited fluctuations of about 20°.

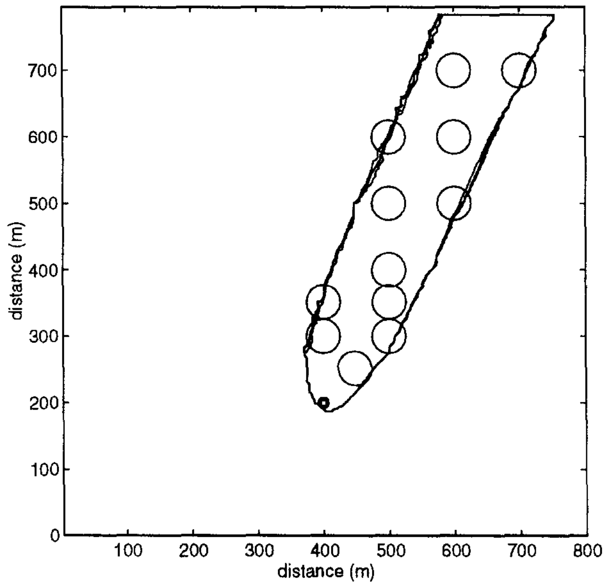

Fig. 20. Thorney Island Trial 13: contours of predicted dose (irregular lines; values 10^4, 10^5, and 10^6 ppm^2 min) and sensors detecting gas (circles); simulation using a wind bearing of 25°. Small square at (400, 200) is the source.

accurately tracks the positions of the sensors that detected gas. Fig. 21 shows the crosswind distance residual analysis. No trend is seen; compare Fig. 19 in which negative crosswind distances were over-predicted and vice versa.

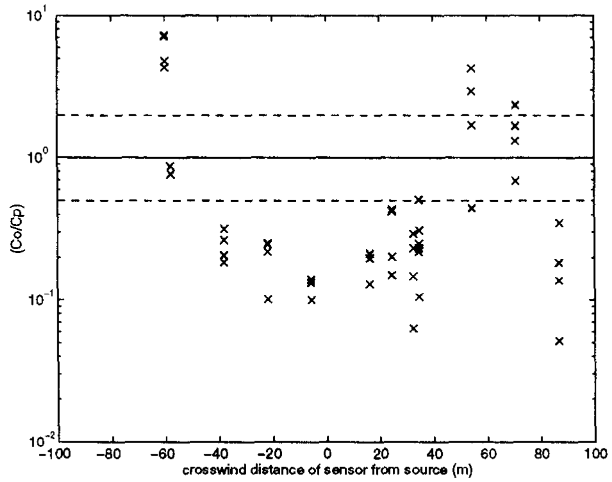

Fig. 21. Thorney Island Trial 13: C_o / C_p as a function of crosswind distance; simulation using a wind bearing of 25°.

9. Summary

This paper has compared the present model with the experimental results from Thorney Island [2], mainly using peak concentrations for comparison. Scatterplots of C_o/C_p against altitude, crosswind distance, and distance from source were presented; no significant trends were found. The most appropriate vertical profile was found to be exponential. Varying the default parameters in the model did not give significantly better agreement with experiment.

In general, about half the predicted peak concentrations were correct to within a factor of 2, and almost all correct to within an order of magnitude.

Parts 1, 2, and 3 of this paper have presented TWODEE, the HSL's shallow layer model for dense gas dispersion. TWODEE uses depth averaged variables to describe the cloud; the shallow water approximations, with extra terms for the leading edge, are used to determine its evolution in time (part 1). The mathematical model is solved numerically using the flux correction scheme of Zalesak; the computer code correctly predicts flow in known test situations (part 2). TWODEE predictions were then compared against large scale experimental data (Thorney Island). Reasonable agreement was obtained when TWODEE was used with the default parameters (part 3).

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