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FITTING BOX MODELS TO THE THORNEY ISLAND PHASE I DATASET

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Summary

It was shown in Carn, Sherrell and Chatwin that a standard least squares procedure could produce very different values for the gravity spread constant A and the advection constant λ in the box model of Picknett, depending on the objective function that was used. This paper examines the difference between the sets of estimates that were obtained from the 5 different objective functions discussed in the previous paper and describes how a cloud envelope can be used to indicate the failure of some sets of estimates to predict the dispersion of the gas cloud adequately.

The problems associated with optimising the empirical constants in the model of Fay and Ranck are also discussed here. The experimental data of Havens and Spicer are fitted to the equation for the radial spread of the gas cloud to estimate the gravity spread constant and this value is used in the subsequent optimisation of the entrainment constants using the Thorney Island data.

Unlike Picknett's model which can be fitted adequately to all the Thorney Island trials, Fay and Ranck's model fails to give a good fit to four of the trials which were conducted at a low wind speed or had an initially high relative density.

1. Introduction

Since van Ulden [1] first proposed the box model to predict the dispersion of a heavy gas cloud in the atmosphere, there has been a proliferation of box models, each one becoming more sophisticated with the physical processes being modelled on a scientific basis rather than ad hoc assumptions. It was apparent at the Second Symposium on Heavy Gas Dispersion Trials at Thorney Island (see other papers in this Volume) that box models are still being produced, with each author concentrating on validating his own model, despite the fact that it may only be very slightly different from a previous one, and without any significant difference in the ultimate predictions. The stage has now been reached when it would seem sensible to validate just a few of the box models with the experimental data (and to exclude the others not because they are not valid but because they have nothing more to contribute than the others) and to come to a general consensus as to how the empirical constants should be estimated to obtain a functional box model which can easily be called upon for future comparisons and predictions.

Each box model contains a number of empirical constants which can vary from as few as four for Picknett's model [2–4] and Fay and Ranck's model [5] to as many as nine for Chatwin's shear dispersion model [3]. A variety of methods have been employed to evaluate the constants [2,6,7]. Carn, Sherrell and Chatwin [8] describe in the second part of their paper how a standard least squares procedure applied to the data from the Thorney Island trials (described in Ref. [9]) was used to estimate the values of the empirical constants in Picknett's model after using several different objective functions. Moreover, it was shown that each objective function can produce a significantly different set of estimates for the empirical constants when using the same experimental data.

This present paper looks at these results in more depth. First of all, various ways of comparing the predictions with the experimental observations are examined with a view to distinguishing between the various sets of estimates that have been obtained. This investigation also includes a consideration of which objective function is most likely to yield the "best" set of estimates (the "best" estimates being judged from the method of comparison used) and whether the function models the physical system and its related variables sensibly. For example, it is explained in Section 3 how the departure times, unlike the arrival times, are not very clear-cut and, therefore, the objective function used should not be too sensitive to variations in the departure times.

It must be emphasized, however, that the values estimated here for the empirical constants in Fay and Ranck's and Picknett's models are not necessarily the final estimates since the models have yet to be fitted to other experimental data such as the Porton Down field trials [2] and Hall's wind tunnel experiments [10–12] which the author plans to do in the future.

2. Selecting those estimates which give the best fit to the Thorney Island data

It has already been explained in Carn et al. [8] how the equation for the cross-section of the cylinder formed two of the objective functions and was also used to predict the arrival time $t_n^{(a)}$ and the departure time $t_n^{(d)}$, according to Picknett's box model, at the nth sensor with co-ordinates (x_n, y_n). For the purpose of this paper, it is sufficient to say that the objective functions are:

$$f^{(1)} = \ln\,(\tau_n/t_n)$$

$$f^{(2)} = \tau_n - t_n$$

$$f^{(3)} = (\tau_n - t_n)/\tau_n \tag{2.1}$$

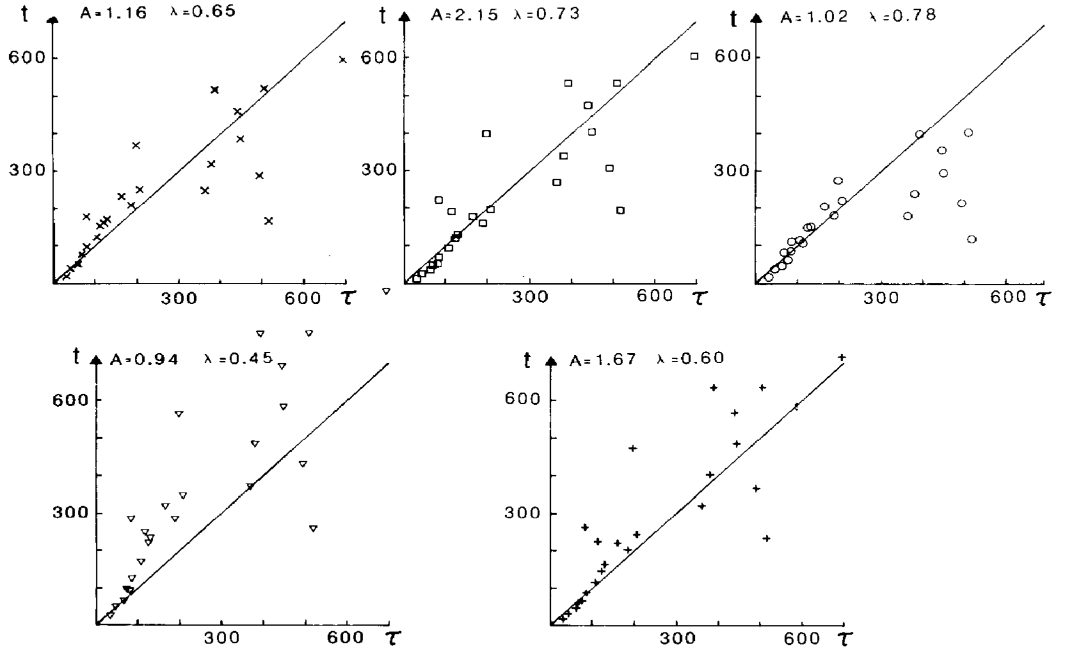

Fig. 1. Plots of data points of arrival and departure times versus theoretical values from the Picknett model for Trial 006 for the 5 measures in eqn. (2.1).

$$f^{(4)} = x_n^2 + [y_n - \bar{y}(\tau_n)]^2 - r^2(\tau_n)$$

$$f^{(5)} = \{x_n^2 + [y_n - \bar{y}(\tau_n)]^2\}^{1/2} - r(\tau_n)$$

where $\tau_n^{(a)}$ and $\tau_n^{(d)}$ are the observed arrival time and departure time, respectively, at the sensor (x_n, y_n), r is the radius of the cloud, and $\bar{y}$ is the distance of the centre of the cloud from the source.
Also, for Pickett's model

$$r^2 = r_0^2 + 2Ab^{1/2}\tau \tag{2.2}$$

and

$$\bar{y} = \lambda\bar{u}\tau \tag{2.3}$$

The two empirical constants being estimated are A, the gravity spread constant, and λ, the advection constant, while r_0 is the initial radius of the cloud, $\bar{u}$ is the mean wind speed at a height of 2 m and b is the constant total cloud buoyancy.

A least squares procedure employing the modified Gauss–Newton algorithm to minimise the sum of squares for each $f^{(i)}$ was used to optimise the empirical constants, A and λ. One method of judging how well the predictions fit the

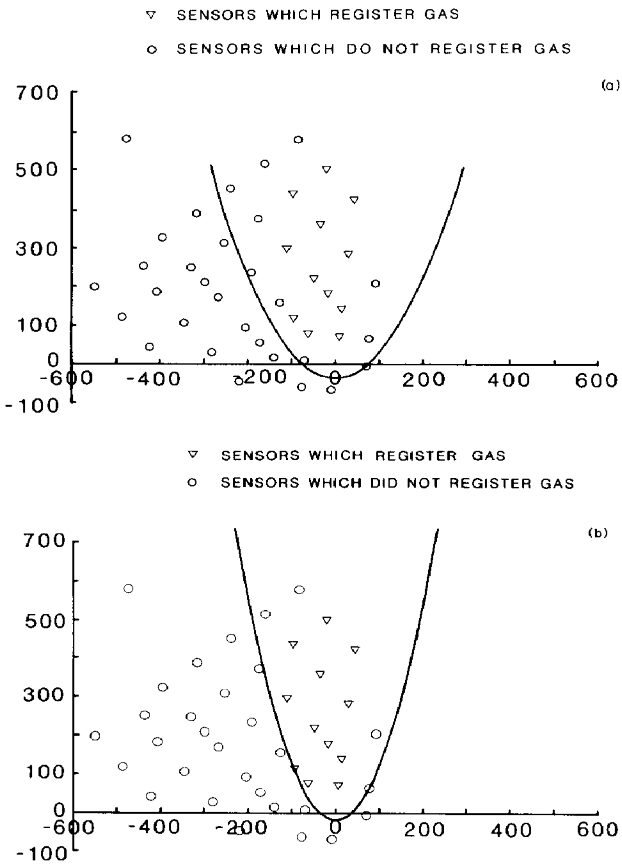

Fig. 2. The predicted cloud envelopes for Trial 006 using the estimates obtained from; (a) $f^{(5)} = [x^2 + (y-\bar{y})^2]^{1/2} - r$ ($A = 1.67, \lambda = 0.60$), and (b) $f^{(3)} = (\tau_n - t_n)/\tau_n$ ($A = 1.02, \lambda = 0.78$).

experimental data is to plot the arrival and departure times predicted using the optimised constants against the actual observed times. Figure 1, taken from Carn et al. [8], shows the observed arrival and departure times from Trial 006 of the Thorney Island trials plotted against the predicted arrival and departure times using the optimised values of A and λ. If a perfect fit was achieved then all the points would lie on the diagonal line $\tau_n = t_n$. However, it was obvious that these graphs did not achieve the purpose of assessing how well the different sets of estimates fitted the data so another method needed to be considered which would distinguish between the various sets of estimates.

One possible solution was to draw the predicted cloud envelope onto a plan of the field on which the trial was carried out along with the positions plotted of those sensors which did detect gas and those which did not. The cloud envelope is made up of those points at which the gas cloud at $\tau + \delta\tau$ intersects the

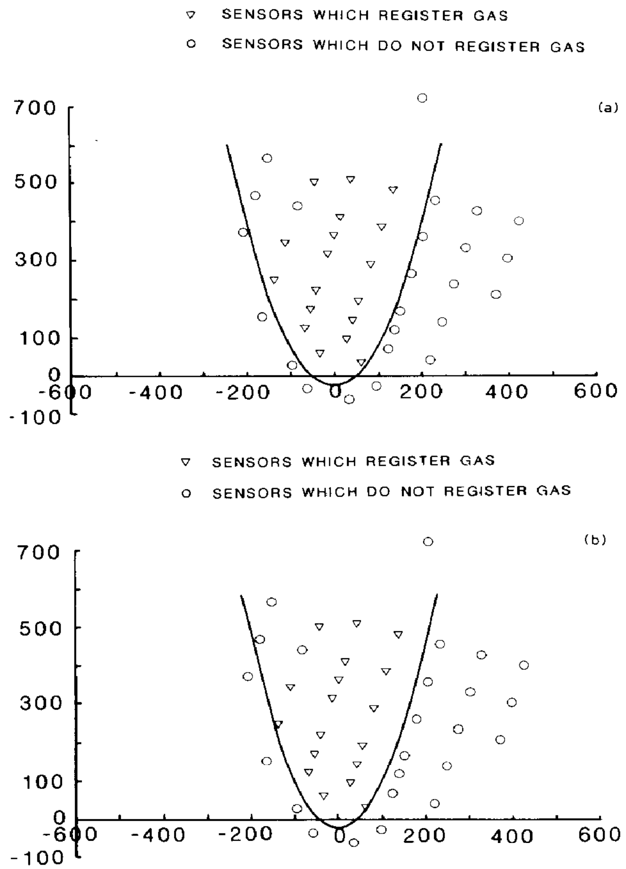

Fig. 3. The predicted cloud envelopes for Trial 008 using the estimates obtained from (a) $f^{(1)} = \ln(\tau_n/t_n)$ $(A=0.99, \lambda=0.72)$, and (b) $f^{(4)} = x^2 + (y-\bar{y})^2 - r^2$ $(A=0.83, \lambda=0.70)$.

circle the gas cloud will have formed, according to Picknett's model, at τ. It is easy to show after some elementary calculus followed by substitution into the equation for the cross-section of the cylinder, that the cloud envelope is given by:

$$x = \pm\left(r^2 - \frac{A^2 b}{\lambda^2 \bar{u}^2}\right)^{1/2}, \; y = \bar{y} - \frac{A b^{1/2}}{\lambda \bar{u}} \tag{2.4}$$

In Fig. 2a, the triangles denote the sensors which detected gas and the circles denote the sensors which did not detect any gas. The co-ordinate system is transformed for each trial so that the y-axis is coincident with the mean wind direction which is assumed to be the cloud path. The values used for A and λ were those obtained from using the objective function, $f^{(5)} = [x^2 + (y-\bar{y})^2]^{1/2} - r$. Obviously the gravity spread constant is too large and/or the advection constant is too small since the parabola is too wide, predicting that the cloud would reach certain sensors when the observations show that it did not.

Figure 2b shows the cloud envelope which gives the most consistent fit with the ground level sensor observations in Trial 006. The values for the empirical constants, which produced this cloud envelope were obtained from the objective function, $f^{(3)} = (\tau_n - t_n)/\tau_n$. Apart from the ground level sensor positioned at (91,204) and the two at (−86,577) and (−163,513), all the other ground level sensors which did not detect any gas fall outside the cloud envelope, which is consistent with the predicted area of ground that saw gas. As for the two ground level sensors positioned at (−86,577) and (−163,513), the concentration of the gas cloud may have fallen below the lower limit of resolution of the sensors by the time the cloud reached these two.

Cloud envelopes were drawn for all of the Thorney Island trials but since the sensor masts were generally spaced up to 100 m apart, it transpired that for some of the trials, more than one objective function would produce estimates which agreed with the observations. Figure 3 illustrates this, where $A = 0.99$ and $\lambda = 0.72$ fit the observations in Trial 008 just as well as $A = 0.83$ and $\lambda = 0.70$. More sensors are required on the right hand side of the field between the line of sensors which detected gas and the line of sensors which did not, before a distinction can be made between the two sets of estimates.

The mean of all the values for A, which produced a cloud envelope that fitted the observations, was 1.12 and the mean of all the values for λ was 0.57. This value for A is in line with the recommendations of other modellers, such as Picknett [2], Fay and Ranck [5] and Wheatley et al. [6], who propose 0.94, 1.00 and 1.07, respectively. This is in contrast to Carn et al. [8] who estimated A to be 1.53 by taking the mean of the estimates obtained from the objective function, $f^{(5)} = [x^2 + (y - \bar{y})^2]^{1/2} - r$. Although $f^{(5)}$ returned fairly consistent values for A, they were generally rather higher than the expected value of order unity.

3. Some comments on the five objective functions

The input data for the objective functions in eqn. (2.1) are the experimental arrival and departure times at the sensors. The arrival time of the cloud at a sensor is taken to be that point at which the lowest sensor on the mast first shows some sign of response to the contaminant, irrespective of the magnitude of the concentration. The measurement of arrival times is generally quite straightforward with no ambiguity, especially for sensors near the source of release; there is usually a definite sharp rise in concentration at a particular time as the cloud first hits the sensor. The departure time, again measured from the lowest sensor on the mast, is taken to be that point when the concentration of the gas "consistently" falls to zero. However, measuring the departure times can be somewhat arbitrary since the cloud edge becomes more diffuse at later times which causes a slow decay in concentration levels and intermittency (hence the use of the word consistently in the previous sentence) along with instrument noise can give rise to further doubt. Care must be taken not to confuse intermittency with measurement noise since the two can produce similar pictures. The author assumes that measurement noise prevails as soon as the sensor gives a negative reading and so the departure time is taken to be that point before the signal fades into measurement noise or when the concentration of the gas consistently registers zero percent.

In view of the somewhat indeterminate nature of the departure times, objective functions should not be too sensitive to variations in the departure times. Consider $f^{(4)} = x^2 + (y-\bar{y})^2 - r^2$, which becomes, after substituting for $\bar{y}$ and r, according to Picknett's box model:

$$f^{(4)} = x^2 + (y-\lambda\bar{u}\tau)^2 - r_0^2 - 2\alpha b^{1/2}\tau \tag{3.1}$$

The rate of change of $f^{(4)}$ per unit change in τ is: $2\lambda^2\bar{u}^2\tau - 2y\lambda\bar{u} - 2\alpha b^{1/2}$. Therefore, as time increases, so does the rate of change of the objective function with respect to τ implying that for later times, the objective function will become increasingly sensitive to variations in the departure times.

A typical dataset taken from the Thorney Island trials will range from an arrival time of 10 s to a departure time of 300 s. However, the objective function, $f^2 = \tau_n - t_n$, will be biased towards fitting the later time since this will lead to a smaller sum of squares (the ultimate aim in the optimisation procedure).

The rate of change of the objective function,

$$f^{(5)} = [x^2 + (y-\bar{y})^2]^{1/2} - r, \text{ with respect to } \tau$$
$$= \frac{-(y-\lambda\tau)\lambda}{[x^2 + (y-\bar{y})^2]^{1/2}} - \frac{\alpha b^{1/2}}{[r_0^2 + 2\alpha b^{1/2}\tau]^{1/2}}$$

This is not such a simple case since the rate of change of the objective function with respect to τ will depend on the position of the (x,y) co-ordinates. For $y=\lambda t$, $\mathrm{d}f^{(5)}/\mathrm{d}\tau$ will decrease for increasing time but if x is held constant (at any value other than when $y=\lambda t$) then $\mathrm{d}f^{(5)}/\mathrm{d}\tau$ will increase.

On the other hand, some simple differentiation will show that for $f^{(1)} = \ln(\tau_n/t_n)$ and $f^{(3)} = (\tau_n - t_n)/\tau_n$, the rate of change of the objective functions with respect to τ decreases for increasing time implying that these two objective functions will be more sensitive to variations in the arrival times than the departure times. This would seem reasonable since the arrival times are fairly well defined. This reasoning is further supported by the fact that $f^{(3)}$ yielded estimates that produced cloud envelopes which gave the best agreement with the observations, for all of the Thorney Island trials except Trials 014, 015 and 018. As yet, no progress has been made with investigating why $f^{(1)} = \ln(\tau_n/t_n)$ did not yield such satisfactory estimates for the empirical constants.

One other point to be considered when estimating the empirical constants is that it is still essential to represent the physics sensibly. The physical system in this instance is the dispersion of a heavy gas cloud and initially the dispersion will be controlled by certain factors such as the negative buoyancy of the cloud. However as time progresses, the ambient conditions will influence the dispersion more than the buoyancy of the cloud and ideally the objective function should reflect the same physical behaviour, by becoming less dependent on A, which controls the gravity spread of the negatively buoyant cloud, for increasing time.

Consider $f^{(4)} = x^2 + (y-\bar{y})^2 - r^2$. The rate of change of the objective function with respect to A is $-2b^{1/2}t$ for Picknett's box model. Similar calculations with $f^{(2)}$ and $f^{(5)}$ show that the modulus of $\mathrm{d}f/\mathrm{d}A$ increases for increasing time implying that these three functions show an increasing sensitivity to A as time increases. It is, therefore, questionable whether these three objective functions are reasonable when optimising the empirical constants of a box model predicting the dispersion of a heavy gas cloud.

4. Optimising the entrainment constants in Picknett's box model

The side entrainment constant c_1 and the top entrainment constant c_2, in Picknett's box model, are related to the volume of the cloud V at time t by

$$\frac{\mathrm{d}V}{\mathrm{d}t} = c_1 2\pi r h \frac{\mathrm{d}r}{\mathrm{d}t} + c_2 \pi \frac{r^2 u_*}{Ri} \tag{4.1}$$

where

$$Ri = \frac{b}{r^2 u_*^2} \tag{4.2}$$

and h is the cloud height, u_* is the friction velocity and Ri is the Richardson number.

The optimisation of the two entrainment constants using the Thorney Island data has alreay been described in Ref. [8].

The value of A used in the optimisation procedure was 1.53 and the mean values of the two constants, c_1 and c_2, were estimated to be 0.68 and 0.24, respectively.

Once again, but this time using the value of 1.12 for A, the two entrainment constants were optimised for the Thorney Island data using a standard least squares procedure and employing the following objective function:

$$f = \ln\left[\frac{CV}{100v_0}\right] \tag{4.3}$$

(The logarithmic form of the concentration equation is used rather than $f = CV/100v_0$ because this prevents the optimisation procedure from overemphasizing those one or two initial concentration readings of 4% and 6% with little regard being paid to the majority of readings ranging from 0.9% to 0.01%.)

The mean values of the estimates of c_1 and c_2 obtained for each of the 14 Thorney Island trials (Trial 005 is excluded since the gas container dropped in two stages) for the side and top entrainment constants are 0.72 and 0.43, respectively. This value of c_1 is similar to that proposed in Ref. [8] and is also similar to the estimates obtained by others validating Picknett's model; in fact everyone appears to be in close agreement over the value of c_1 whereas c_2 has been evaluated for a wide range of values with some very small estimates such as 0.15 and 0.14 which were suggested by Picknett [2] and Brighton [13], respectively.

The solid line on each graph in Fig. 4 shows the predicted concentration values using the estimates obtained from optimising just the trial data while the dashed line shows the predicted concentration values using the mean values for the entrainment constants. It can be seen that in the cases illustrated, optimisation with the data alone leads to a good fit with the Picknett model despite the scatter of data in some cases as in Trial 016. The predictions obtained using the overall mean values are encouraging except for Trials 009, 012, 017 and 019 where the predicted concentration levels are too low. These four trials were conducted at a low wind speed and/or had an initially high relative density. The wind speed, initial relative density and other initial conditions are given for some of the trials in Table 1 to illustrate the difference between the four trials (009, 012, 017 and 019) and the others [9].

5. Fitting experimental data to Fay and Ranck's model

Optimisation of the four empirical constants in Fay and Ranck's model has not been so straightforward due to the way the advection of the heavy gas cloud was modelled. In this box model, the advection speed of the cloud is assumed to be equal to that given by the logarithmic wind profile at a fixed fraction of the cloud height:

$$\frac{\mathrm{d}\bar{y}}{\mathrm{d}t}=\frac{u_*}{\kappa}\ln\left(\frac{\beta h}{z_0}\right) \tag{5.1}$$

where β is the advection constant, z_0 is the roughness height and $\kappa(\approx 0.4)$ is von Karman's constant.

This equation for $\mathrm{d}\bar{y}/\mathrm{d}t$ must be integrated numerically so an analytical expression cannot be derived for the predicted arrival and departure time at a sensor in the field. Thus the three objective functions $f^{(1)}$, $f^{(2)}$ and $f^{(3)}$, are not immediately usable for optimising the empirical constants in Fay and Ranck's box model. (In theory, these three objective functions could be used if numer-

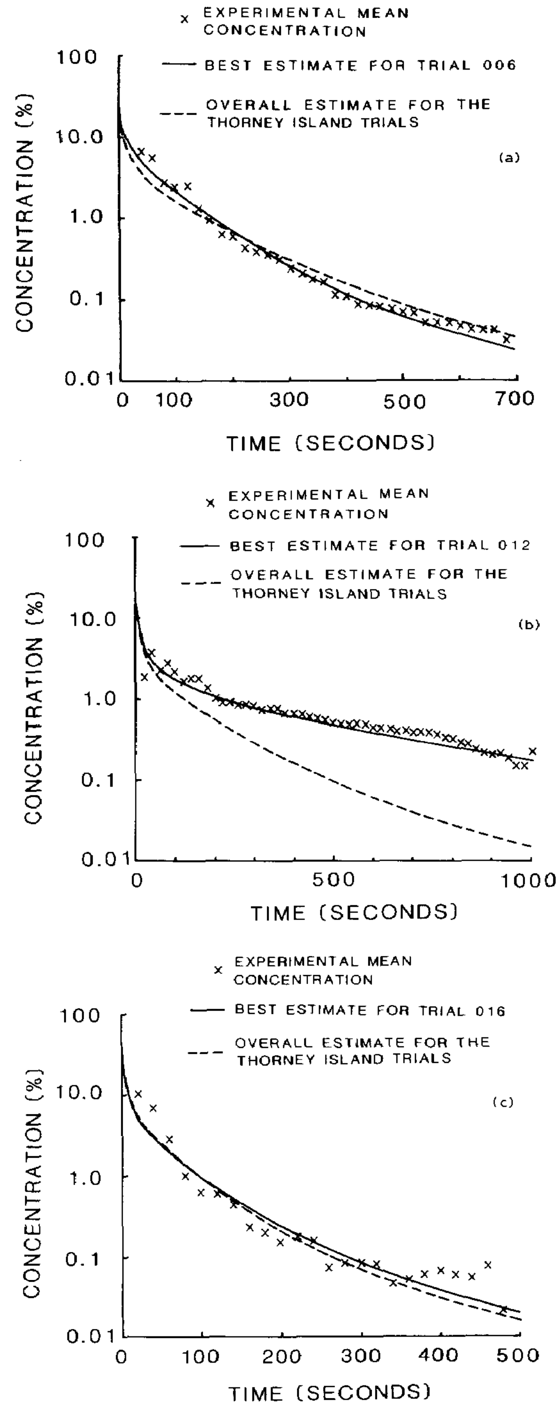

Fig. 4. Comparison of data from 3 Thorney Island trials with Picknett's box model.

TABLE 1

Summary information for seven Thorney Island trials

	Trial						
	006	007	009	012	016	017	019
Wind speed at 10 m in m s^{-1}	2.6	3.2	1.7	2.6	4.8	5.0	6.4
ρ_0	1.6	1.75	1.6	2.37	1.68	4.2	2.12
Ri_0	9.0	9.3	26.5	25.2	3.0	13.8	3.7
Pasquill stability category	D/E	E	F	E	D	D/E	D/E

ical methods were applied but the computational time would be very long since the equation for $d\bar{y}/dt$ has to be integrated numerically several times as a hit or miss method is used to calculate each predicted arrival or departure time.)

Another problem arises when $f^{(4)}$ or $f^{(5)}$ is used to optimise A and β. Since $d\bar{y}/dt$ is dependent on h, the height of the cloud, the expression is also, therefore, dependent on the two top entrainment constants which need to be assigned appropriate numerical values. Optimising the entrainment constants first does not overcome this problem since the expression for the volume is also dependent on A, the gravity spread constant, which would normally take the value obtained from minimising the equation to the circle. Two ways of overcoming this problem are:

(1) To optimise the two entrainment constants and the gravity spread constant altogether using eqn. (4.3) and then optimise β.

However, this optimisation procedure yielded nonsensical values for the three constants. For example, one particular run of the procedure returned a value of 0.04 for A and a negative value for one of the entrainment constants. In fact, values such as these can produce predictions similar to the experimental concentration readings except for those initial one or two data readings. Due to the way the data from the Thorney Island trials has been presented in the hardcopy books, the concentration readings can only be satisfactorily measured every 20 s, so the first reading will be at 20 s for most trials, although in some cases the first reading was measured at 40 s. Thus a tentative conclusion as to why this procedure fails is that the concentration data is too sparse in the initial stages of the release.

(2) Another possibility would be to optimise the objective functions, $f^{(5)}$ and f in eqn. (4.3) simultaneously using both the observed arrival and departure times and the mean concentration data.

This technique has still to be perfected, so in the meantime, the value of 1.05 has been taken for A. This value was obtained from optimising the equation for the radius of the cloud using the data from the 66 trials carried out under calm conditions by Havens and Spicer [14]. Fay and Ranck ignore side entrainment and, therefore, only consider top entrainment. The top entrainment is defined as a function of the local Richardson number which gives a continuous transition from dispersion dominated by the negative buoyancy of the cloud to dispersion influenced by the ambient conditions

$$\frac{\mathrm{d}V}{\mathrm{d}t}=\frac{\pi r^2 u_* c_1 c_2}{[c_2^2+c_1^2(b/r^2u_*^2)^2]^{1/2}} \tag{5.2}$$

Using a standard least squares procedure with eqn. (4.3) as the objective function, the two top entrainment constants were optimised for each of the 14 Thorney Island trials. The mean of the 14 estimates obtained for c_1 and c_2 were:

$c_1=0.32$, $c_2=15000$

Provided $1/c_2 \ll 1$, the value of c_2 is more or less irrelevant when fitting the model to the Thorney Island data. However, the model needs to be fitted to other datasets before any judgement can be made about the role of c_2 since it mainly affects the concentration levels in the initial stages of the release (i.e. for high values of the Richardson number) when the data are often sparse as was the case in the Thorney Island trials [8].

The results for the three trials, 006, 012 and 016, are shown in Fig. 5. Again, the solid line represents the predicted concentration values using the estimates obtained from optimising the data for that individual trial, while the dashed line represents the predicted concentration values using the mean values over all the trials for the entrainment constants.

A good fit was obtained with Fay and Ranck's model when the estimates particular to that trial were used except for Trials 009, 012, 017 and 019. A comparison with Trial 012 in Fig. 4 shows that Picknett's model gives a much better fit when using the estimates optimum to that trial. Fay and Ranck's modelling of the entrainment of air is the same as the expression for top entrainment in Picknett's model when $g'h \gg u_*^2$ [8]. So a tentative conclusion to be made about the poor fit with Fay and Ranck's model, especially in the earlier stages of release for those four trials, is that it is due to the omission of side entrainment. To see whether this is actually the case will require optimisation of a side entrainment constant along with the optimisation again of the two top entrainment constants since these two coefficients will no longer have to compensate for the exclusion of side entrainment.

6. Comparison of the Picknett and Fay and Ranck models

Figure 6 shows a comparison between the predictions obtained from Fay and Ranck's model and those obtained from Picknett's model with both models taking the mean values for the empirical constants. Since the mean values did not give a good fit to Trials 009, 012, 017 and 019 for either of the box models,

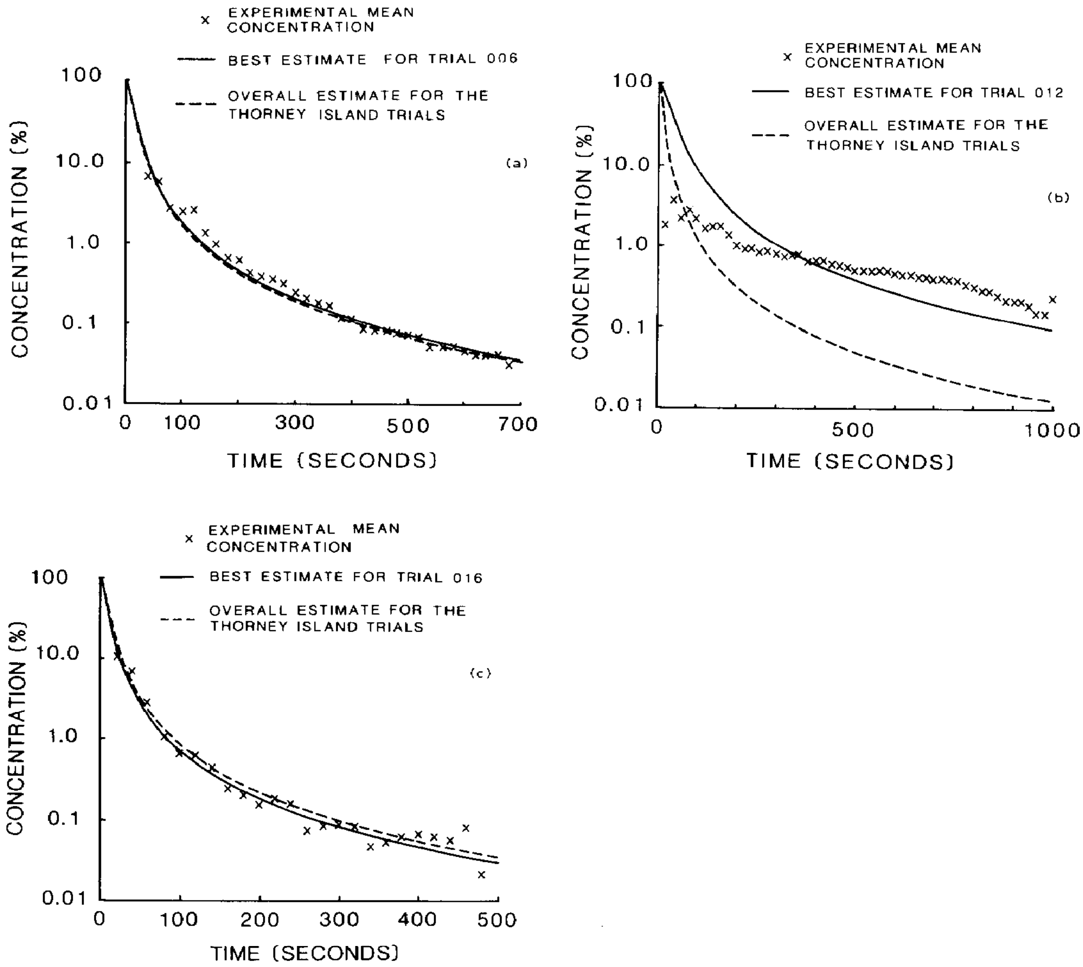

Fig. 5. Comparison of data from 3 Thorney Island trials with Fay and Ranck's box model.

these four trials are not included in the comparison. Despite the different structure of the two models, either model fits the data equally well. However, Picknett's box model will remain the first choice since it can give a good fit with all the Thorney Island trials, unlike Fay and Ranck's model which gives a disappointing fit in some cases even after optimising with just the data particular to that trial.

7. Conclusion

This work still leaves many questions unanswered but progress has been made which should pave the way for future research. Firstly, it is apparent that the values of the estimates can differ considerably depending on the objective

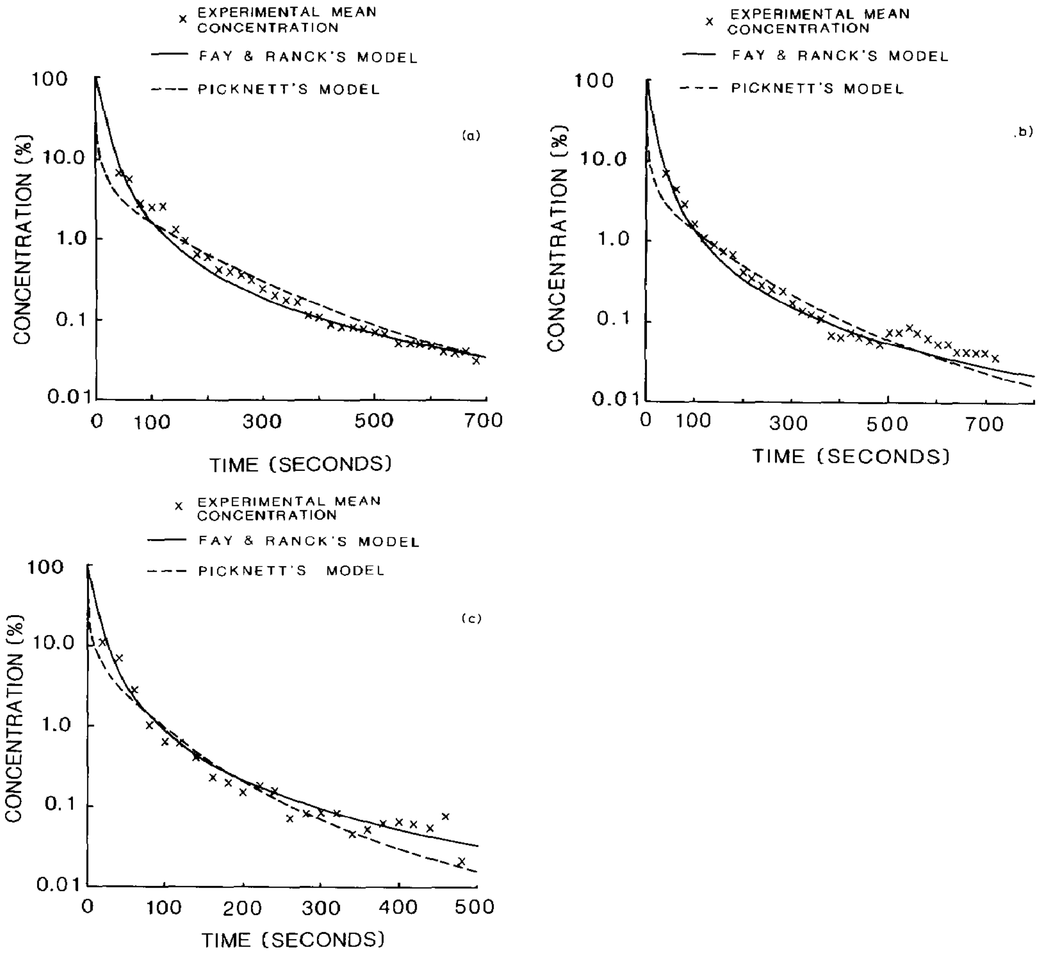

Fig. 6. Comparison of data from 3 Thorney Island trials with Picknett's and Fay and Ranck's models. (a): Trial 006, (b): Trial 007, and (c): Trial 016. —— Fay and Ranck's model: $A=1.05$, $c_1=0.32$, $c_2=15000$. --- Picknett's model: $A=1.12$, $c_1=0.72$, $c_2=0.43$. × experimental mean concentration.

function used (sometimes referred to as the goodness of fit measure) which Wheatley et al. [6] and Carpenter et al. [7] also discuss. The work also highlights the importance of exploring other methods such as the use of cloud envelopes, which might expose any systematic (or otherwise) deviation of the predicted values from the observations which may not be apparent when using another method of comparison as was the case for the fit-observation diagrams illustrated in Fig. 1.

The real test of a box model is its ability to predict all possible release scenarios. Apart from a possible failure to model certain physical aspects of dispersion such as the omission of side entrainment in Fay and Ranck's model, the merits of a model will also depend on the optimisation of the empirical constants. Taking the mean of the estimates which describe individual trials does not ensure good predictions for certain releases even if they were included in the original ensemble. Wheatley et al. [6] use a sophisticated numerical method to estimate the overall optimum constants and the same method was applied to the individual estimates the author obtained for the Thorney Island trials, but the results were disappointing. There appears to be few references, either in the literature of numerical analysis or that of modelling heavy gas dispersion, on how to estimate the overall optimum constants after a mathematical model has been fitted to a number of trials. This subject would seem worth pursuing since it is an essential part of modelling.

I am grateful to the referee for his valuable contributions, which have a strong statistical basis, on how to improve and continue this work. So far, the statistical nature of this analysis has been neglected and the author intends to rectify this by considering the possible application of a variance-stabilizing transformation to justify the use of a uniform weight least squares procedure. Another suggestion from the referee is to compute confidence intervals for each trial, and if there is a reasonable degree of overlap then it would be acceptable to optimise all the trials at once.

8. Acknowledgements

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