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METEOROLOGICAL OFFICE
BOUNDARY LAYER RESEARCH BRANCH
TURBULENCE & DIFFUSION NOTE

T.D.N. No. 159

Estimates of Uncertainty in Dispersion Modelling.

by Dr. F.B.Smith.

October 1984.

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SUMMARY

Risk assessments associated with releases into the air of any potentially hazardous material (such as radionuclides, toxic or inflammable gases) must involve not only the expected air concentration, deposition or dosage but also the uncertainty involved in such expectations.

This paper briefly examines the errors that arise from the models and their associated parameters, from the numerical methods employed, from the inexactness or inappropriateness of the basic meteorological (and other) input data, and from the inherent variability of the atmosphere arising from its turbulent character.

It goes on to consider how these errors affect the pattern and magnitude of the downwind groundlevel hazards in subtle but often dramatic ways. It emphasises that on-site measurements of meteorological parameters should be made with proper regard to the scales of the advection-diffusion processes involved, and not over some quite arbitrary and unrelated time-scale as is often the case at present.

1. General aspects of uncertainty

A release of any gaseous or particulate species into the atmosphere is subject to many processes which involve uncertainty. The uncertainty may arise from fundamental ignorance (complete or partial) of the physical and chemical processes involved, from a lack of information about the circumstances under which the release took place, from an inability to extract the most information from the input data that is available (perhaps because computer facilities or required time may be limited or non-existent), and from the inherent variability that is always present in a turbulent medium such as the atmosphere. These areas of uncertainty are summarised in Table1

Generally the greatest area of uncertainty arises from a lack of information concerning the input data to models. The input data can be divided into data on emission characteristics, data on the state of the atmosphere, and data on the underlying terrain. The first of these includes the source strength (how much material has been released in total and how did the release rate vary in time), the buoyancy associated with the release and the velocity of the release-gases (both of which influence the rise of of the plume), where the release into the atmosphere took place (from a stack, from ventilation vents, from near the ground etc), and the physical and chemical character of the release (the particulate size distribution, the decay or reaction rates, etc). This source of uncertainty may be the greatest for accidental releases of radionuclides at nuclear plants, especially during the first few days following the accident until a detailed survey of what actually happened is available. Uncertainties of an order of magnitude may be expected which will therefore swamp all other uncertainties.

Usually uncertainty on the state of the atmosphere will be the next largest. However, how important this will be in practice will depend very much on what aspect, or consequence, of the release has to be modelled.

For example whether or not a fixed community will be, or has been, affected by a plume during a 24 hour continuous release is decided much more easily and reliably than trying to estimate the concentration at a given fixed place at a specified time. In other words the uncertainty depends on whether we are concerned with air concentrations, total dosages or ground depositions, whether we are concerned with specific point values or ranges of values over a large area, whether at a given time, or at any time during a period, or an integrated time-average, and whether we are dealing with a specific release or a possible release some time in the future.

It is obvious that the more data are available, the more facilities are at hand to extract meaningful information from the data, the less specific one is required to be in terms of time and space, the more accurate one can hope to be in one's estimations.

2. Field and laboratory evidence for uncertainty

(i) Winds and trajectories

Perhaps the most fundamental question of all is "Is this receptor affected by the plume or not?", and the answer, whatever it is, automatically provokes a second question "how certain are you that the predicted path of the plume is realistic?". Clarke et al.(1) has studied 32 tetroon releases which have lasted for more than 250km or 12 hours travel time in various Environmental Protection Agency (EPA) field experiments. They compared the trajectories of these tetroons with trajectories determined by various meteorological trajectory models. The model giving the best overall results was the National Oceanic and Atmospheric Administration's Air Resources Laboratory Atmospheric Transport and Dispersion (ATAD) model. With this model, the tetroon trajectory could be expected to be 8 - 10 % of the trajectory length to the left of the diagnosed position, with a standard error of about 25-30% of the trajectory length. In terms of time of travel T the mean separation e between the tetroon position and the diagnostic position was given approximately by:

$$|e| = 0.8\,T \quad \text{(km)} \qquad (3 < T < 21\text{hrs})$$

and the standard deviation $\sigma(|e|)$ just slightly less than this. The errors were thought by Clarke et al. to be probably less in well-defined flow patterns and whenever meteorological data (especially radiosonde data) were available more frequently than every 6 hours. In situations when likely plume trajectories need to be forecast ahead for the following hours (for example as soon as a hazardous emission commences) the extra uncertainty associated with forecasting future meteorological states will increase the probable error. The magnitude of the forecast error depends very much on the sophistication of the model used and, in particular, on the details of the boundary layer representation and its resolution. It also depends quite critically on how the gridvalues (which can often show small-scale roughnesses) are spatially smoothed. No proper analysis has yet been done on these errors, perhaps because of the difficulty in formulating a totally satisfactory comparison.

However as a first stage in determining the quality of forecast trajectories based on the output of the Meteorological Office's so-called fine-mesh operational numerical weather prediction model (15 levels in the vertical, horizontal gridlengths at 50°N of 68km north-south and 83km east-west), Maryon and Riggs have recently compared trajectories starting from the same point at the same real time, one based on an initial actual field but subsequently on the model's forecast fields, and the other entirely on forecast fields based on a run starting 12 hours earlier. The following differences were found:

	median	mean	standard deviation	mean distance
after 24hours	91km	106km	76km	600km
after 36hours	174km	219km	141km	1200km

The expected difference is thus about 1/6th of the distance of travel and is therefore comparable to the error found by Clarke between ATAD trajectories and tetroon trajectories. There is clearly room for a lot more basic research in this area.

(ii) Plume rise

In models that have been tuned to give the correct mean plume rise at downwind distances exceeding 800 metres, the expected difference between predicted and observed rise is about 13% of the total plume height, according to field studies by Moore (2). Leahey and Davies (3) have studied plume rise from a flare made visible through the injection of oil into the flame. The rise h' was generally consistent with the theoretical prediction that $h' \propto x^{2/3}$ until final rise was attained. However the correlation coefficient between 777 observed and theoretical plume rises measured over 2-3 minute periods was only 0.74, i.e. the root mean square expected error is roughly 2/3 the r.m.s variation in plume rise over the 777 observations.

Willis and Deardorff (4) have studied plume rise within a laboratory convectively-mixed layer. They show that active convection has a profound effect on plume rise, indicating the need to modify Briggs' (5) well used formula in these conditions. They also studied the effect of a fluctuating horizontal wind but unfortunately their paper fails to give an indication of the resulting scatter.

(iii) Ground-level concentrations

There are so many variables that govern the concentration of a species emitted from an upwind source that it is difficult to define an absolute measure of uncertainty. In general the uncertainty has to be linked to a specific model which contains only a limited number of parameters. The spread of concentrations measured when these parameters are apparently nearly the same yields the uncertainty for that model for that set of parameter-values. But the problem of doing this is clouded by the sensitivity of the model to possible errors in the inferred parameter-values, and discussion of this point will be left till later.

To give but an example of the uncertainties experienced in practice, Crawford (6) has shown that for a specific hour and at a specified receptor point within 10km of the source when the intervening countryside is flat and the meteorological conditions are steady, the ratio of the predicted concentration to the observed, in which the former is determined using a basic Gaussian plume model, can vary from 0.1 to 10 : a rather large measure of uncertainty!

Vanderborght et al. (7) have made measurements of aerosol concentration and deposition around a metallurgical plant in Belgium over a 14-month period, together with reliable data on emission rates and local meteorological conditions. They claim that a bi-Gaussian model provides predictions that give short-term concentrations which are generally within 40% of the observed, and average depositions within 60%. Comparing this with Crawford's result it is clear that the quality and detail of the input data have a marked effect on the output accuracy.

Harrison and McCartney (8) made ground-level measurements of NO_x concentration 1.2km downwind from five 46m high stacks at a fertilizer factory, and found reasonably good agreement with the predictions of a simple Gaussian plume model using conventional Pasquill-type stabilities and σ_z. For all stabilities the predicted values lay within $\pm$ 50% of the observed values, but with a tendency for the former to be higher than the latter, especially in unstable conditions.

On a much longer time-scale, Simpson and Jakeman (9) have shown that annual maximum acid levels at 2 stations vary around 3 to 4 over a ten year period, due almost equally to inter-annual variations in the wind-field and to variations in emissions and other meteorological factors.

(iv) Concentrations within plumes

Deardorff and Willis (10) have studied both buoyant and non-buoyant plumes within a laboratory convectively mixed layer. They find that concentrations do vary within plumes and that the cumulative frequency distribution of non-zero sampled concentrations is virtually log-normal. When meandering of the plume, and resulting occasional zero concentrations are included, the mean square concentration fluctuation $\overline{C'^2}$ is found to vary very little across the time-mean plume but decreases significantly with downwind distance, partly because a given receptor is more consistently either totally within the plume or out of it. Fackrell and Robins (11) have made similar experiments in a simulated neutral boundary layer. They find $\overline{C'^2}$ is a maximum at $z/h = 0.75$ for a ground level source (h is the mean-concentration half-height) which presumably has a very small contribution from vertical plume meandering. Elevated sources give profiles of $\overline{C'^2}$ with only a single maximum, the height of which approaches that of the ground-level source as the two mean-concentration profiles approach each other at large downwind distances. Again $\overline{C'^2}$ is shown to decrease substantially with downwind distance. The actual magnitude of $\overline{C'^2}$ depends not only on x,y and z but also on the period of sampling.

(v) Plume widths σ_y and σ_z

The variability of width depends again on the way meteorological conditions are parametrized. On a single occasion when all the mean-flow parameters are by definition fixed, σ_y and σ_z will vary in time due to spatial and temporal variations in turbulent energy on many scales. Smith and Readings (12) have looked at a specific single day in unstable conditions in summer and showed that in the micrometeorological part of the spectrum the energy levels in narrow frequency bands (corresponding to averaging times t_a and sampling times $2t_a$) showed considerable scatter: the root mean square variations of the levels were about 60% of mean levels. This degree of variability would also be reflected in plume widths averaged over $2t_a$, at distances downwind from the source where an equivalent Eulerian averaging of t_a seems appropriate.

Moreover when different occasions with apparently the same mean-field characteristics are grouped together, width-scatter is generated not only from the inherent variability in the turbulence but also from more subtle differences between the occasions.

The National Council on Radiation Protection and Measurement NCRP Report No.76 (13) quotes data on lateral width, σ_y, in which widths measured in field experiments over flat terrain are compared with predictions on the basis of a stability classification expressed in terms of the vertical temperature lapse rate. To define stability in this way is questionable, and this is perhaps one reason why the scatter (90% of the points lie within a factor of 4) is so large. Values of width (measured and predicted) found in the experiments carried out in the more complex terrain at Mt. Iron are also given in the Report. Here classification was made, not in terms of lapse rate, but in terms of wind direction fluctuations. Apart from a few very wild outliers, the great majority of points are now within a factor of 2 in the comparison of measured to predicted, showing that in spite of the rougher terrain the parametrization was more realistic.

The Report also quotes Briggs and McDonald's (14) analysis of σ_z inferred from ground-level measurements made in the Prairie Grass Experiment By proper parametrization, in which σ_z/L is expressed in terms of $u_* x/(UL)$ (where L is the Monin-Obukhov length scale and u_* is the friction velocity), the scatter of σ_z is reduced to within a factor of about 2 in both stable & unstable conditions out to $x < 10\, U|L|/u_*$.

Observations of plumes emanating from sources close to the ground on top of buildings suggest that the character of gusts, associated with incursions of faster moving air from greater heights, is very important to the spread at short range. A sudden gust causes a rapid alongwind convergence and a compensating lateral divergence of the plume. The rate of spread can then be linked to the sharpness of the gust "front", an aspect which is not explicitly considered in normal atmospheric diffusion theory, but which is commonplace in aerodynamic theory.

3. Sources of Uncertainty

Table 1 sets out the major sources of error and uncertainty in dispersion estimation. The first and most obvious source is in the nature of the models themselves. They are only simplified models of the real world They are designed to reflect our limited scientific understanding of what is actually taking place, to meet certain specifiable objectives, which may differ from model to model, to be expressible in terms of a limited input-data supply, and to be capable of yielding results with available resources (manpower, time and computer facilities). An individual model may work well within a certain range of conditions for which it was designed but relatively badly outside this range. For example a Gaussian plume model may be satisfactory in rather uniform flow over level terrain, but may work poorly in strong shear flow over irregular terrain.

Many dispersion models have an element of parametrization, that is when some aspect of the physics or chemistry involved in the process being modelled is represented by some approximate algebraic or empirical expression which may include one or more adjustable constants. Sometimes these parametrizations yield solutions whose properties are in some respect physically unacceptable. For example, solutions of the classical eddy diffusion equation are known to give unrealistic plume widths close to the source, except when it is at ground level. Other parametrizations are in danger of being just too simplistic. For example it is clearly perilous to represent the often complex consequences of stability in the boundary layer by a single stability parameter as is usually done through necessity. Moreover many models contain parameters which cannot be measured directly in the atmosphere but have to be inferred indirectly or represented empirically with consequent loss of precision.

The actual solution of model equations can generate errors either by mathematical instabilities or by having too coarse a resolution. The former can nearly always be overcome with care but the latter are more insidious and can generate totally artificial dispersion of plumes and clouds for example unless very deliberate steps are taken to prevent this.

All models depend on input data, and these data may be insufficient, unrepresentative or erroneous. Data may be insufficient for assessing the possible consequences of future accidents and their associated probabilities This is particularly true for meteorological data in which so many scenarios are possible. In general at least 10 years reliable data are required to provide a reasonably representative data set. Rare conditions which lead to extreme concentrations or depositions are usually very difficult to quantify and may require even longer data sets.

The problem of representativeness is one of the biggest "headaches" facing anyone setting up meteorological instrumentation near a source of potentially hazardous material. The source is usually on or near large buildings, the local terrain is often heterogeneous and consequently all atmospheric properties, such as wind speed, are varying significantly from place to place. There is no simple solution to this problem since there is no single place which is representative of the changing conditions affecting the plume as it advects downwind. Faced with this dilemma, perhaps the best one can do is to site anemometers and windvanes in a nearby meadow with the maximum uniform fetch in every direction at a height of 10 metres, or, if the fetch is good at a height corresponding to half the stack height. Meteorological observing stations, whilst maintaining good quality instruments, may be too far away to give an adequate picture of local flow conditions, even in flat countryside. Vanderborght et al.(7) have given results which emphasise this from a study of wind speed and direction differences between sites at Beerse and Mol separated by some 22km on the very flat northern Belgium plain. The standard r.m.s. differences were about 15° and 2 ms^{-1}.

It must be stressed that all meteorological instruments should be properly maintained and recalibrated faithfully at intervals recommended by the manufacturers. More robust instruments require less maintenance of course but may lack responsiveness in certain critical conditions, for example in light winds.

Finally, careful consideration should be given to systems which will present meaningful and useful information to the appropriate person clearly and quickly in the case of an accidental release. Raw data from a windvane for example could be quite misleading and certainly confusing under such circumstances. Suitably averaged values of windspeed and direction, and turbulence levels, should be immediately available with the aid of a dedicated data-processor. The details of the data averaging and sampling should be linked to the safety issues involved and not to some arbitrary standard time like 1 hour.

Having said all this, it would be inappropriate not to remind ourselves that in spite of all these potential sources of error, the largest source of error, especially in accident situations at nuclear installations is likely to be associated with the amount, duration and type of release.

4. Sensitivity to errors and inherent variability

(i) It is often assumed that the mean values of the various parameters appearing in a model algorithm are the most appropriate, and these will give the best estimate of the mean concentration. This is clearly not so. For example if the Gaussian plume model were to be applied to dispersion from a source near ground level and it was known that the wind speed was fluctuating rather slowly between 3 ms^{-1} and 7 ms^{-1}, say, with a uniform probability distribution over the range, then $\bar{u} = 5$ ms^{-1} and, if no other parameter varied in this fictitious scenario, since $C \propto 1/u$, the value of C calculated using $\bar{u}$ would underestimate the true average C by some 6%. This is fairly small admittedly, but if the plume were also buoyant, the effect of the fluctuating wind on plume rise and hence on downwind ground-level concentrations would be much greater. Edwards and Misra (15) have studied this point. They consider the effect of mesoscale horizontal wind fluctuations on the effective entrainment rate of ambient air into a buoyant plume, and hence on its total rise. From their results it is easily shown that if $\bar{u} = 10$ ms^{-1} and $\sigma_u = 2.5$ ms^{-1}, and the average final virtual source height is 500m then the maximum ground level concentration is likely to vary tenfold in response to the fluctuations in u from about $6\bar{C}$ in strong "gusts" to about $0.77\bar{C}$ in relative lulls. ($\bar{C}$ is the maximum concentration assuming a single steady 10 ms^{-1} wind speed $= \bar{u}$).

To sum up it is important to remember that concentrations do not depend linearly on the basic input parameters, and that some of the parameters may be essentially inter-correlated.

(ii) As Sykes (16) points out, any measure of concentration within a plume is a time-averaged sample from a stochastic field. There is therefore a random component to the measurement which depends on the statistical properties of the instantaneous concentration field. He shows that the reduction in the variance s_T of the mean concentrations evaluated over a series of periods of duration T, as T increases, depends not only on T/T_e, where T_e is the Eulerian velocity timescale, but also on the variance s_o of the instantaneous concentrations, and on the mean concentration $\bar{C}$. On the centreline of a highly intermittent plume, Sykes shows that for large T:

$$\frac{s_T}{\bar{C}^2} = \frac{T_e}{T} \ln\left[1 + 2\frac{s_o}{\bar{C}^2}\right]$$

By "intermittent" Sykes means the plume is meandering about the long-term centreline, sometimes covering the receptor and sometimes not. Gifford (17) was the first to provide a useful theory of fluctuating plumes in his classic and still very important paper of 1959.

Draxler (18) has studied ^{85}Kr air concentrations measured at 13 sites located 30 to 150 km from the source at the Savannah River Plant in South Carolina, over a two year period. Comparing these with a long-term sector average Gaussian dispersion model which takes into account the varying meteorology, he showed that the root mean square error e of ratios of observed to calculated concentration (or calculated to observed, if the latter is smaller than the former) for different averaging times ranging from 1 week to the full 2 years, took the following values:

averaging time	1 wk	1 mth	3 mths	1 yr	2yrs.
e	5.2	3.6	2.6	1.8	1.7

Venkatram (19) and Hanna (20) have also studied the magnitude of concentration fluctuations within a plume. Hanna shows that the ratio of the standard deviation σ_c of these fluctuations to the mean concentration $\bar{C}$ varies across the plume and increases towards the edges since the entrainment of "clean" ambient air around the edges means σ_c decreases more slowly than $\bar{C}$ as one moves away from the centreline. Hanna also quotes measurements made near to 50m - 100m high stacks in which the concentration showed peak-to-mean values around 50-100 at the ground, and values 1-5 at the same level as the source. At much greater downwind distances $\sigma_c/\bar{C}$ appeared to vary like (L/σ_o) , where L is the Eulerian length-scale and σ_o the virtual size of the plume at the source.

Venkatram has shown that the standard deviation of the natural log of the concentration $\sigma(\ln C) \propto (u^{-1/2} z_i^{1/6} h x^{-1})$, in a convective boundary layer, where z_i is the mixing depth and h is the height of the source (assumed greater than $0.1z_i$). Deardorff and Willis (10) confirm the quite rapid fall-off of concentration variance with downwind distance x in their measurements of buoyant and non-buoyant plumes in water tank experiments.

(iii) Smith and Readings (12) and Venkatram (19) have both considered the effect of a non-zero mean vertical velocity during the time of plume sampling on the ground level concentration. Smith and Readings do this very simply by looking at turbulence records on a single convective day and inferring the magnitudes of the vertical velocity associated with appropriate sampling and averaging times, and show that on this one occasion the 10-minute concentration 1200m downwind from a 100m stack would be expected to vary by some 15% (s.d.) about the mean due to this cause. Venkatram considered the problem from a theoretical standpoint and showed that the standard deviation would increase with stack height and decrease with downwind distance.

Smith and Readings also considered the sensitivity of the ground-level concentration on this day to variations in other parameters. As found by others, the variance increases with lateral distance from the centreline of the plume, with fluctuations in u (here $\sigma_c \sim \frac{1}{3}\bar{C}$), and with fluctuations in small-scale σ_w which only produced $\sigma_c \sim 0.03\,\bar{C}$.

(iv) Increasing the averaging time decreases the variance of any stochastic quantity such as concentration. NCRP Report No.76 (13) summarises the findings from many field measurements over flat terrain and in many stability conditions in terms of ranges in the ratios of observed to predicted concentrations, the latter based on Gaussian plume models. Figure 1 is a rough attempt to integrate these results. If R is defined as that number for which 90% of the observed concentrations within the plume lie within 1/R and R of the predicted concentrations, then the Figure expresses R as a function of distance downwind x and averaging time T.

(v) It was mentioned earlier that to gain adequate meteorological data measurements need to be made over at least 10 years. A study by Simpson and Jakeman (9) emphasises this point. They have attempted to link observed daily SO_2 concentrations at various sites in Newcastle, Australia, to wind speed. They show that they can explain about half the range of the annual maximum daily-SO_2 concentrations over a 10-year period (the maximum concentration varies by a factor of about 3-4) in terms of an inverse relation between SO_2 concentration and wind speed, and a log-normal probability distribution for the latter. The remaining variation they link to variations in emissions and other meteorological factors.

(vi) Finally in this section, the effect of rainfall must be mentioned. For any species that is removed by rain the inherently variable and patchy nature of rain can generate very irregular air concentration fields and deposition patterns. To predict the statistics of such patterns is made difficult for example by the complex air motions within clouds, and as a result of our lack of total knowledge of how radionuclides and other species are incorporated into raindrops. In a long-term statistical sense variations in single rain-event deposition at any point due to emissions from a constant source may be linked most strongly to variations in rainfall amount (which of course can vary by two or three orders of magnitude). In practise on any one occasion the problem is often to know where rainfall occurred and how the moving plume experienced the moving rain system. These are major problems.

5. Conclusions

We have attempted to review some aspects of modelling uncertainty. The review does not claim to be anything like exhaustive however. Emphasis has been placed on the following needs:

(i) to assess inherent variability and its consequences, whenever possible.

(ii) to take into account fluctuations in the meteorological input data (even when the time-mean value may be zero).

(iii) to make meteorological measurements close to the source over as uniform a site as can be found, and with full appreciation of appropriate sampling and average times, and to make this information available in a simple and clear way to Safety Officers in real time.

(iv) to improve models, reducing systematic errors.

(v) to assess input data errors and biases, whilst recognising that inherent errors may be unavoidable, especially in modelling future scenarios.

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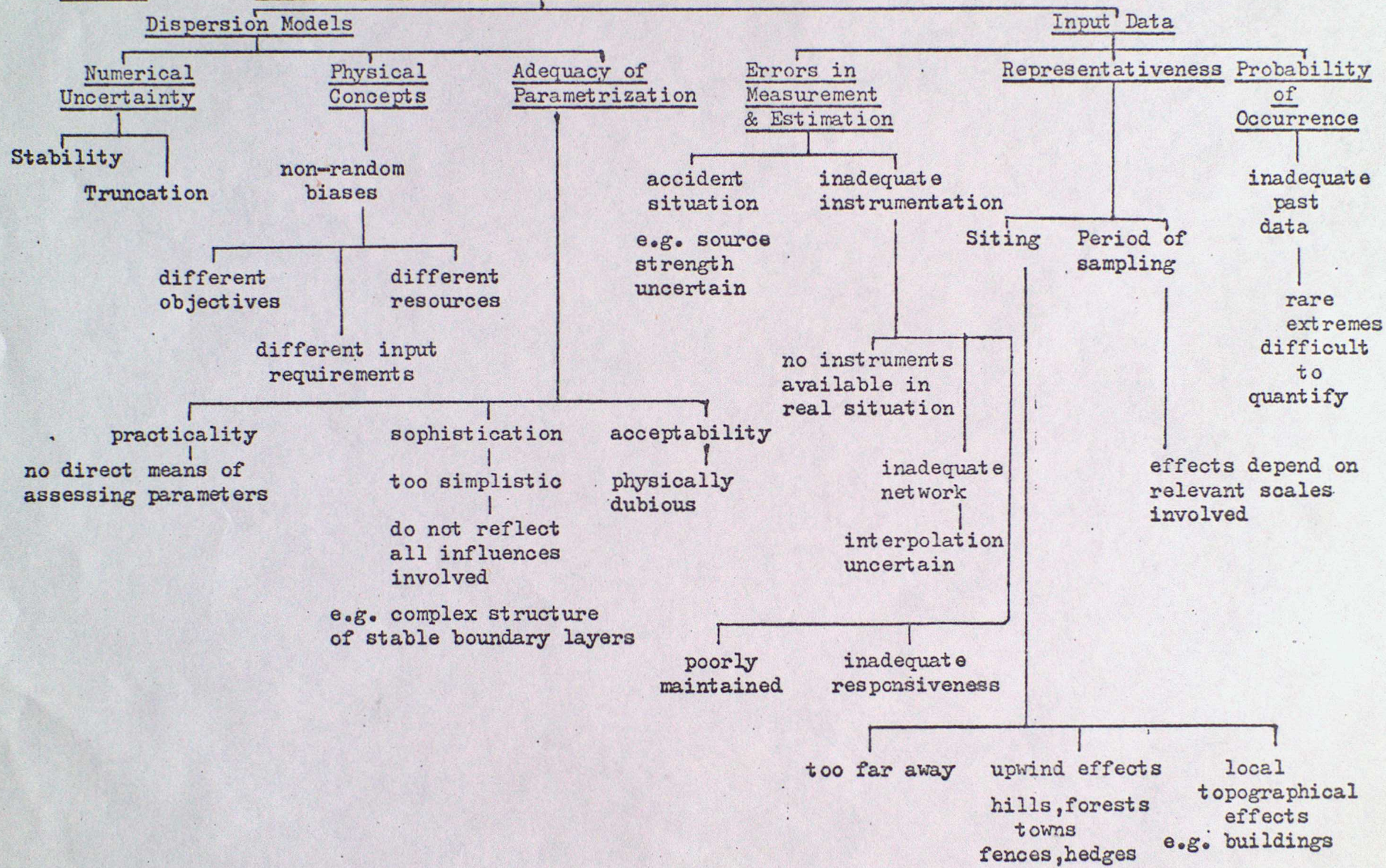
TABLE I Uncertainty in Model- Predicted Concentrations



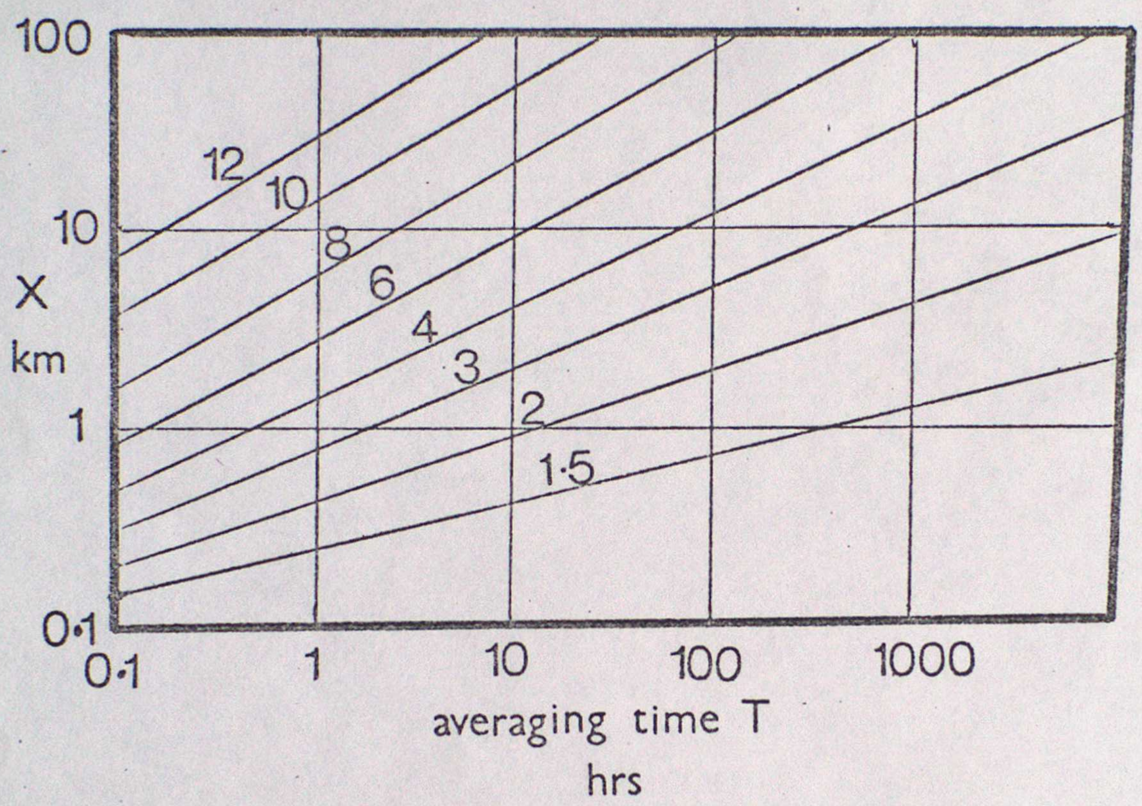


Figure 1. Contours of the scatter parameter R for a non-buoyant plume, under all stability conditions over a flat plain. Using Gaussian models, 90% of observed data will lie within 1/R and R of the predicted data.