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**THE PREDICTION OF PESTICIDE
RESIDUES IN CROPS BY THE OPTIMUM
USE OF EXISTING DATA**

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The prediction of pesticide residues in crops by the optimum use of existing data

Abstract

The commitment of large resources to the provision and evaluation of data on pesticide residues in/on crops makes it vital to optimise the value of existing extensive information. Variations in the many (sometimes uncontrollable) factors which determine pesticide deposits on crops and their subsequent dilution and disappearance make the consideration of pesticide residues and the estimation of maximum residues levels an inexact subject. A knowledge of these factors and their variability can reduce, or at least modify, the current regulatory requirements for expensive formal residues trials, which often have considerable limitations, both in their execution and in their interpretation. Information required for the successful prediction of pesticide deposits and residues at harvest is discussed and summarised in a recommended stepwise approach to the consideration of pesticide residues in crops.

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1 INTRODUCTION

The importance of reliable quantitative information on the levels of residues arising from the use of pesticides has increased considerably in recent years. The principal interest has always been focussed on the evaluation of the toxicological significance of pesticide residues in the food supply of man and his animals. However, with the increasing concern over the environmental effects of agrochemicals, emphasis is also being placed on evaluating the significance of pesticide residues in the food supply of birds, fish and other non-target wildlife species.

Since the initial deposit of a pesticide and its subsequent residues may move or be transported, it is important to consider all pesticide residues within the context of their relationship to the total environment.

The estimation of maximum residues levels found in food and feed following maximum registered uses and their subsequent conversion into legal limits (maximum residues limits or MRLs) commits large resources, both in manpower and funds. Industry is required to provide a large data base and government is expected to evaluate

this, setting MRLs, monitoring residues in the food supply and the environment and reassuring the public about the significance of any residues found.

Traditionally, data from residues trials have provided the mainstay of the assessment of hazards from pesticide residues in food. Few attempts have been made to predict residues levels as a preliminary step in evaluating hazards to consumers or to optimise the value of the extensive data base on pesticide residues which already exists. In addition, there appears to be a general lack of appreciation of the wide use that can be made of information on the factors that affect the initial deposit of a pesticide during application and the subsequent disappearance of that deposit and its residue, both in food crops and in the environment.

This report outlines the factors affecting the initial deposit and its subsequent disappearance, discusses the role and importance of formal pesticide residues trials, the options for extrapolations and predictions and recommends a stepwise approach to the consideration of pesticide residues in crops.

Residues in crops at harvest may result from -

1. uptake by the plant of soil-applied pesticides or otherwise occurring in the soil
2. translocation of pesticides applied to the plant before the edible part of the crop has formed
3. applications when the edible part of the plant is already present

Residues at harvest from the first two circumstances are usually low and often below the limit of determination. Since the majority of significant residues at harvest result from 3, the emphasis in this report is on the application to crops when the edible part of the crop is already present.

2 THE INITIAL DEPOSIT

2.1 Application and crop factors affecting the initial deposit

The efficacy of a pesticide application in controlling a pest or disease is usually governed by the amount of a pesticide - containing spray deposit that is present, its distribution and, in some cases, the coverage of the plant surface achieved. There is an ever-increasing emphasis on the need for more efficient deposition of pesticides, that is, the same or improved degree of control with less toxicant. For this reason, much attention has been given in recent years to the physico-chemical factors which govern the physical nature and distribution of a pesticide deposit after the toxicant has reached the treated surface. However, the physical factors that are involved in the transport of the pesticide to the target surface also require careful examination. All these were considered in an excellent review by Ebeling (ref.1) and much of this is still relevant.

Pesticide residues occurring in crops at harvest depend on two factors:

- i. the initial deposit, its distribution and coverage and
- ii. its disappearance after application, both apparent through dilution by crop growth, and real, through the effects of various physical, chemical and biological activities.

With adequate knowledge of these, a preliminary estimate of the residue level at harvest can be based on this information alone, reducing the need for formal residues trials, which should be used with the preliminary estimate to estimate the maximum residue at harvest. Normally a review of data from extensive formal trials is required to establish MRLs but the planning and extent of such trials can be strongly influenced by competent estimates of expected residues.

Some factors which affect the initial deposit are those which contribute to the definition of the proposed use (Fig.1). Thus the description of the registered uses should normally include:

- the formulation details
- the rate of application (ai/ha)
- permitted application equipment
- volume applied

Other factors determining the deposit are the physical properties or characteristics of the treated crop itself. These include:

- weight of the crop
- surface area/weight ratio of the crop
- the nature of the crop surface
- degree of interception of the spray by the crop

Meteorological conditions will also affect the size and distribution of the deposits.

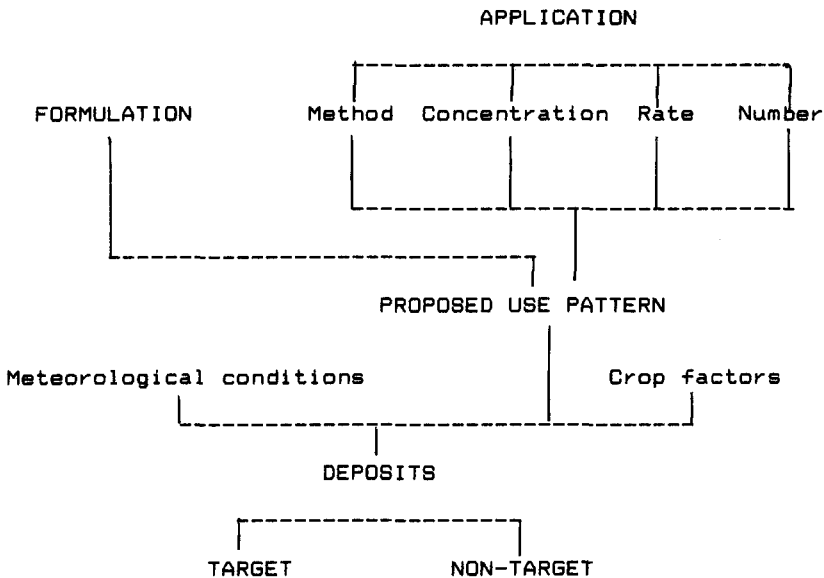


Fig.1. Factors affecting the initial deposit

The rate of application of a pesticide clearly dictates the upper limits of a deposit which can possibly occur on a target or subsequently in a harvested crop. An insecticide applied uniformly at 10 g/ha to an apple orchard expected to yield 20 metric tonnes of apples per ha would result in a residue not exceeding 0.5 mg/kg even if all the applied insecticide was found in the crop at harvest. Similarly a pesticide applied at 1 kg/ha to a crop yielding only 2 tonnes/ha could result in a maximum residue of 500 mg/kg if all the pesticide was found in the crop at harvest.

Fig.2 indicates the ranges of maximum residue levels that could be anticipated by comparing rates of application with average commodity yields from treated crops. Obviously these theoretical maximum deposits are never achieved in practice for many reasons.

The quantity of a pesticide actually deposited and the uniformity of its distribution depend to a great extent on the equipment used for its application. 'Spray quality' (the distribution of droplet sizes in the spray) can be adjusted so that the droplet spectrum is optimum for a particular target crop. Usually the elimination of large and very small droplets in a spray will increase target deposition and improve efficacy.

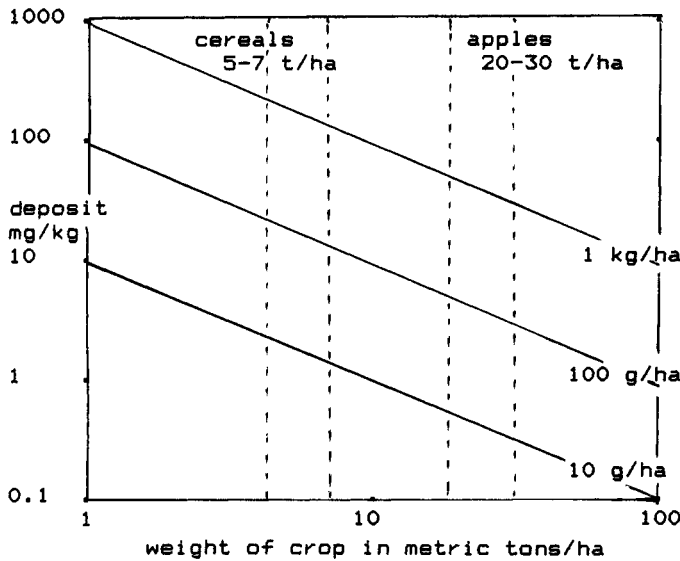


Fig. 2. Ranges of theoretical maximum deposits of pesticides in relation to average crop yields.

Although most of the studies of the deposits of various droplet sizes on plant surfaces have been concerned primarily with the efficacy of the toxicant for pest and disease control, an appreciation of the factors which govern deposits is also of great importance in the evaluation of residues data. The careful selection of formulation and application equipment can contribute to more uniform deposits which can make the task of evaluation of residues that much more definitive.

Even though the edible part of the crop may not be the target for the application, whenever present it will intercept some of the spray and its characteristics will affect the deposit. Information is not readily available on many relevant factors such as the ratio of leaf surface to total weight for leafy vegetables and the increment of growth or weight increase for all crops in the last few days or weeks before harvest. However, estimates of deposits on certain fruit can be made if certain reasonable assumptions are made. Fig. 3 shows the relative surface area of some fruit crops per unit weight (compared with apple = 1) assuming that the fruit are spherical and weight equals volume for all fruit. Because of differences in size between varieties and crop ages, the presentation is only an approximation but it clearly illustrates the use that can be made of such a comparison in evaluating the significance of reported deposits.

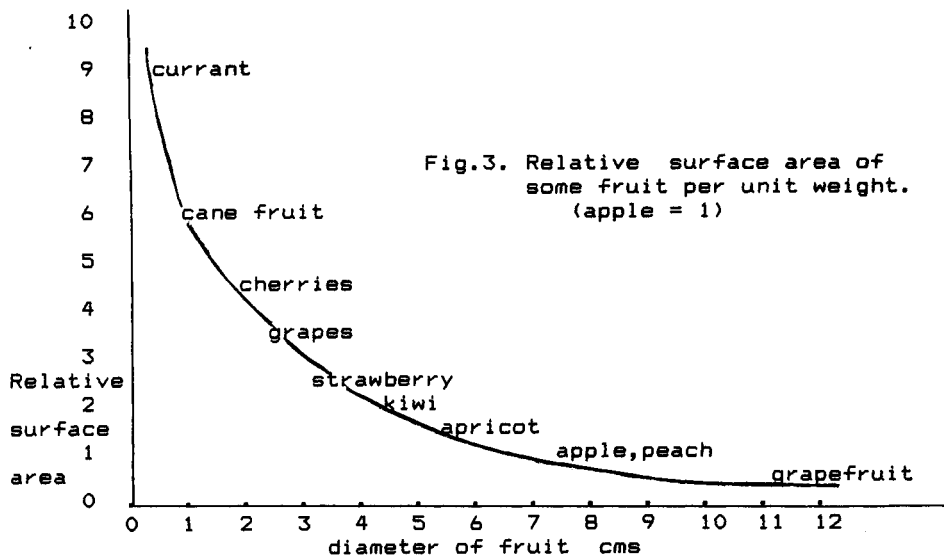


Fig. 3. Relative surface area of some fruit per unit weight. (apple = 1)

Thus for equal applications, deposits on grapes can be expected to be about x3 the deposit on apples on the basis of higher surface area per unit weight. The nature of the fruit surface also plays a role in retaining the initial spray and deposits on furry or hairy skins, e.g. peaches or kiwis will be higher than on smooth or waxy skins.

Since deposits are usually reflected in the residue at harvest and therefore in MRLs, it is to be expected that the differential in deposits will be demonstrated in MRLs for a pesticide. A study of a range of Codex MRLs for a number of non-systemic pesticides on apples and grapes shows expected trends for some but not for all.

TABLE 1. Comparison of some Codex MRLs for apples and grapes

Pesticide	apples	grapes	ratio
azinphos-methyl	1	4	4:1
dichlofluanid	5	15	3:1
flucythrinate	0.5	1	2:1
thiophanate-methyl	5	10	2:1
vinclozolin	1	5	5:1
permethrin	2	2	1:1
carbaryl	5	5	1:1
dicofol	5	5	1:1
chlorobenzilate	5	2	1:2.5
deltamethrin	0.1	0.05	1:2
fenvalerate	2	1	1:2

The comparisons in Table 1 suggest that there could be anomalies in the data used to estimate some of these MRLs since rates of application were comparable in most cases. Further study of national and international MRLs in the light of these observations could contribute to rationalisation and harmonisation of MRLs.

Data on initial deposits are essential to the complete evaluation of pesticides residues data.

2.2 Initial deposits observed in practice

In many formal residues trials which concentrate on residues at harvest, little attention is paid to the initial deposit. There is often little or no evidence that the toxicant was, in fact, ever present on the crop. Thus to evaluate residues at harvest in perspective when direct application is made to the edible parts of the crop it is essential to have information on the initial deposit, or residue at day 0. The overall distribution of pesticide deposit may be extremely variable under some circumstances, for example on individual apples in an orchard following a commercial application (ref.2). Such variability in the deposit can lead to a wide range in the residues in primary samples at harvest. If the residues data are to be used for the estimation of maximum residue levels, then the sampling programme at harvest would need to very carefully planned so that the data are suitable for the intended purpose.

Hoerger and Kenega (ref.3) reviewed many aspects of pesticide deposits and correlated representative data in an attempt to derive a basis for predicting residues levels. Data on initial deposits from more than 250 different pesticide/crop combinations were studied and reasonable guidelines were developed for the prediction of residue levels in certain crops before data from formal residues trials become available.

In Table 2, for each crop grouping, the upper limit represents an estimate of the highest level of initial deposit, calculated on the basis of applications of 1 kg/ha. (The original table was on a basis of 1 lb/acre). The figures used were weighted towards extreme levels found and included data following multiple applications but their paper made no reference to variability resulting from the possibly wide range of sampling techniques.

TABLE 2. Upper limits and typical limits for deposits of pesticides on crop groups. (Based on ref. 3)

	Initial Deposit mg/kg for 1 kg/ha applied		
	upper limit	typical limit (mean)	approx ratio upper/mean
Grass	110	92	1.2
Forage crops (alfalfa, clover)	58	33	2.4
Leaves and leafy crops	125	35	3.5
Cereal grains	10	3	3.3
Whole pods with seeds	12	3	4.0
Fruit	7	1.5	4.6

However, for many purposes, Hoerger and Kenega considered that the typical limit (mean) values would be more useful than the upper limit.

As expected, for more uniform crops such as grass and forage, the ratio upper/mean limits is close to 1, whereas the ratio is much higher for crops such as fruit where the deposits on individual fruit can vary considerably. This emphasises the importance of a full understanding of the sampling techniques employed especially when the crop sample consists of a limited number of large fruit (ref.4).

A recent study has been made of the initial deposits of a number of pyrethroid insecticides on a wide variety of crops reported in the Evaluations of the FAO/WHO Joint Meeting on Pesticide Residues from 1979 to 1989. The deposits reported depended to some extent on sampling techniques, crop development stage and variations in the portion of crop sampled. However, using the approach of Hoerger and Kenega the estimates of upper limits of deposits were generally in accord with Table 2. Most of the pyrethroid data followed low rates of application and the use of modern spray equipment and this, together with some variations in the range of crops considered, might well explain the differences in the two sets of estimates. The estimate of the upper limit also depends on the interpretation of the data available and the method of selecting the limit.

For lettuce and some other leafy crops, the upper limit for deposits was 60 mg/kg for 1 kg/ha applied; for small fruit the upper limit was 20 mg/kg for 1 kg/ha applied; for large fruit the upper limit was 13 mg/kg for 1 kg/ha applied. These are four to ten-fold extrapolations since the maximum rate of application of most pyrethroids does not exceed 250 g/ha; the estimated upper limits for deposits at practical application rates were -

lettuce and spinach	15	mg/kg
small fruit	5	mg/kg
large fruit	3	mg/kg

Fig.4, based on a composite of the above estimates, indicates the ranges of maximum deposits that can be expected on a number of crops from current practices in a range of application rates. These reflect the relative surface areas of the fruit crops although the deposits on the smaller fruit are not as high as predicted from the surface area comparisons. The general listing of the fruit as 'deposit collectors' is not definitive and further studies are necessary. Fig.4 can be used to identify those residues trials where the initial deposit was outside the expected range, suggesting that the application technique or other factors affecting the deposit did not adequately represent good agricultural practice. The average expected deposit is about 50% of the maximum indicated in Fig.4.

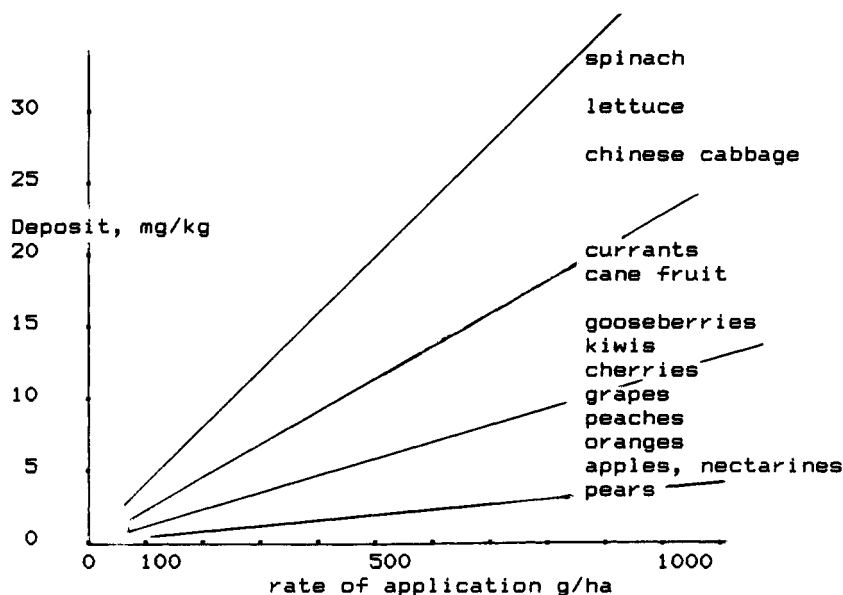


Fig. 4. Ranges of maximum deposits on some crops predicted from existing data.

It is difficult, if not impossible, to isolate and determine the significance of individual factors in influencing a pesticide deposit. However, other than the rate of application, those most likely to have the greatest effect on actual deposits namely -

- spray quality (application equipment)
- crop characteristics and degree of crop interception
- meteorological conditions

reflect, in some respect, the decisions of the farmer or applicator on how and when to spray and in what conditions. They are not controllable by design of the pesticide product or registration. This suggests that continuing demands of registration authorities for the repetition of formal residues trials with all new pesticides adds very little to the already vast data base on pesticide residues which already exists. A much more rewarding research programme would measure deposits, comparing application equipment and crop interception to add to the basic information on factors that determine pesticide residues.

3 FACTORS AFFECTING THE FATE OF A DEPOSIT

3.1 Post-application factors

The characteristics of the formulated product which are important in determining the quantity and quality of the deposit can also contribute to the prediction of environmental behaviour.

Formulations are usually designed to optimise performance and minimise operator risks but they can also influence the persistence and bioavailability of a pesticide residue. Methods of application and choice of equipment are closely associated with the type and properties of the formulation. Information on these aspects is important in the estimation of deposits on a crop, the identification of the probable sites of deposition in the environment and the subsequent fate of the deposit.

The fate of pesticide on or in a crop can usually be predicted successfully from the physical/chemical properties of the compound and data on mobility and fate in plants derived from laboratory studies (ref.5). It should be recognised that the crop is only part of the environment in which the pesticide is applied. Since it is the specific target of the application, deposits on-target are expected to be higher than deposits off-target although the reverse has often been claimed to be the case.

On the surface of the plant the deposit is exposed to a variety of environmental conditions and may be lost by rainfall, volatility, oxidation, hydrolysis or photodegradation. Within the plant, metabolism is the only significant mechanism for reducing the concentration of the pesticide. These post-application factors vary and are not controlled by man.

Requirements for pesticide registration include a number of physical and chemical properties which are important in the prediction of the general behaviour of the pesticide and its likely stability and reactivity as a chemical and influence the mobility and disappearance of a deposit. These include -

- vapour pressure
- solubility in water
- partition coefficient between water and an appropriate non-miscible solvent such as n-octanol
- chemical, photochemical and biological stability
- adsorption/desorption characteristics

These properties are usually supplemented by studies on the metabolism of the compound in a selected range of relevant crops. Before complete analytical methodology for residues can be developed it is necessary to know the composition of the terminal residues. The use of radio-labelled pesticide compounds is usually the only satisfactory way of providing such data (ref.6).

3.2 Prediction of loss of a deposit

From the information on the formulation and the application of a pesticide and a knowledge of the crop characteristics, together with the use of previous data, it is possible to estimate the initial deposit on the relevant edible part of the crop. A consideration of factors affecting the fate of this deposit will then give a qualitative estimate of the residue at harvest.

An estimate of the maximum residue at harvest is often reflected in the maximum residues limits or MRLs established by national governments or international agencies following the evaluation of formal residues trials. In a number of cases however, even though maximum registered uses are used in the trials, other aspects of good agricultural practice may not have been followed, or the method of application may not have resulted in a maximum deposit. In particular, where the MRL has been based on data from only a few trials, the estimate and hence the MRL can be in error. In such cases the qualitative prediction may provide a better estimate than one derived from the results of limited trials, particularly if the trials were of poor quality in execution and reporting.

3.3 Predicting pesticide residues disappearance by modelling

Although very few authors have studied the existing extensive data base on pesticide residues, a number have examined the effects of one or more specific factors affecting the disappearance of residues and attempted to correlate these with the resultant residues. Several have proposed mathematical models for the prediction of the disappearance of pesticide residues on growing crops.

Leffingwell et al (ref.7) estimated the effect of temperature on ethion and 'Zolone' residues on citrus foliage; Thompson and Brooks (ref.8) studied the effects of temperature and rainfall on the disappearance of a number of organophosphorus compounds on citrus foliage. Under field conditions Van Dyk (ref.9) observed the effect of sunlight on parathion residues but not the effect from rainfall or temperature, although such an effect was observed under laboratory conditions.

Staiff (ref.10) could not correlate average weekly temperature with the degradation of parathion on the foliage of apples or peach trees. Nigg et al. (ref.11) showed good correlation for ethion persistence on citrus foliage with heating degree days, rainfall and leaf wetness, both alone and combined with time. Nigg et al. (ref.12) reviewed the use of weather variables to explain the disappearance of pesticide residues observed by different research groups. In this review, mathematical models were presented for predicting the disappearance of residues as a general approach to regulatory problems but these do not seem to have been adopted or developed further. In succeeding papers Nigg and co-workers demonstrated the applicability of the time/weather disappearance models (ref.13).

The most commonly proposed mathematical model for pesticide residue disappearance is the first order rate equation

$$\frac{dN}{dt} = -kN$$

where k is the disappearance constant and N the mass present at time t . From this equation the well-known half-life equation $t_{1/2} = 0.69/k$ can be derived.

Sutherland et al. (ref.14) in the report of 'the half-life working party' listed three objections to the first order rate equation based on time alone.

1. The half-life concept has no basis in reality in the case of the disappearance of pesticide residues from growing crops since the disappearance is an accumulation of a number of causes.
2. The extrapolation of a straight line function for any time other than a short period cannot be justified.
3. The generalisation cannot be made that a given pesticide on a given crop will always disappear at the same rate.

In order to overcome the objections to the use of the 'half-life concept', several authors have used multiple linear regression models to predict the disappearance of pesticide residues. Nigg et al. (ref.11), Spinu and Iwanowa (ref.15) and Stamper (ref.16) have proposed models and claimed some success in demonstrating their validity. Timme, Frehse and Laska (ref.17) tested 420 series of residue decline experiments and found that the apparent first order model provided the best fit for 35% of the cases. They suggested some simple transformations enabling the use of linear regression for the calculation of residue levels at a given time and the confidence interval for the mean residue. They found that the transformation referred to as 'first-order root function' provided the best fit for additional 35% of the cases. In spite of the relative success of Timme et al, a study of these models and their applicability, leads to the general conclusion that at present there is no well-defined model of universal application to the successful prediction of the disappearance of pesticide residues on crops.

In view of these difficulties, perhaps a more general pragmatic approach would be more rewarding. The expected maximum residue at harvest, on which the MRL is based is determined by the three 'd's - deposit, dilution and disappearance and these are related by

$$\text{maximum residue at harvest} = \underline{D} \times \underline{d1} \times \underline{d2}$$

where \underline{D} = maximum expected deposit

$\underline{d1}$ = dilution factor which allows for crop growth in the period between application and harvest and would therefore be governed by the pre-harvest interval (PHI)

$\underline{d2}$ = disappearance factor which takes into account the properties of the compound and time and the climatic conditions between application and harvest

The use of this approach is recommended in the Annex to this report. However, more information is needed on the weight increases in crops in the later stages of growth so that dilution factors can be expressed accurately.

In spite of the objections to the 'half-life' concept and the difficulties in representing disappearance under a wide range of conditions from a wide range of surfaces by a single figure, the disappearance factor, d_2 , must clearly be time-related and an approximation of practical use. It must also be separated from the effects of crop dilution since much of the published information on 'half-lives' includes crop growth dilution and this may account for some of the variations reported. In the absence of all the information needed to arrive at a best estimate of d_2 , an average 'half-life' could be used or the approach of Timme et al developed further.

4 DATA FROM RESIDUES TRIALS AND ESTIMATION OF MAXIMUM RESIDUES LEVELS

For many years formal, supervised residues trials have formed the basis of most national and international estimates of maximum pesticide residues in crops at harvest. The use of these alone presents a number of pitfalls for the unwary. Data obtained from trials are necessarily limited by practical considerations since it is impossible to cover all the variety of conditions of soil, climate, farming practices, etc, under which a pesticide may be used on a crop.

Even if trials are carried out according to strict guidelines (ref.19) in order to eliminate as many variables as possible, there are still post-application factors which are not controllable by man. These include the climate which governs the rate of growth and ripening process of a crop and thus the time of harvest.

Therefore, although well-planned trials will model practical pesticide applications, unless a sufficient number of trials are carried out and emphasis is directed towards the identification of conditions and factors that lead to the highest residues following registered uses and other 'good agricultural practices', the required residues data will not be forthcoming. There is ample evidence from the activities of enforcement agencies around the world that a number of MRLs have been based solely on inadequate trials data. As a result, shipments of otherwise acceptable food commodities have been rejected because they contained pesticide residues that exceeded MRLs which apparently excluded some 'good agricultural practices' not encompassed by the formal trials. To obtain the maximum value from any experimental data, it is essential to design the residues trials to obtain data of the highest quality which can be used with confidence in subsequent evaluations.

Thus the major role of supervised trials should be to confirm, reject or modify the predictions made from the extensive data already available and to define more clearly the upper end of the range of residues expected at harvest when the pesticide is used in agricultural practice. Data from limited trials should never be used on their own, since this could lead to an erroneous estimate which is unrealistic.

The principal role of MRLs in enforcement activities should be to monitor compliance with registered uses. Therefore it is important to ensure that all residues resulting from all legitimate registered uses are covered by an estimate of the maximum residues level. This is particularly important when the monitored commodity is supplied from a number of different countries where, for sound biological reasons, both the pre- and post-harvest factors affecting deposits and their disappearance can vary considerably.

5 POSSIBILITIES FOR EXTRAPOLATION

It is clearly not practicable to carry out supervised trials

- a) on all of the many varieties and cultivars of crops,
- b) on all the crop species on which a pesticide may need to be used
- c) under a wide range of climatic conditions and cultivation techniques.

Since so many aspects of trials cannot be adequately controlled by man, the design and scope for such comprehensive trials would be far beyond any reasonable requirements for data. Indeed it is difficult to see what relevant new scientific information could be obtained from such studies.

Thus the concept of extrapolation is essential to the evaluation of residues data and the estimation of maximum residues levels. Extrapolation of actual data can be used to estimate residues on other crops, varieties and cultivars grown in situations and circumstances different from those in which the original data were generated.

The Codex Committee on Pesticide Residues (CCPR) and the FAO/WHO Joint Meeting on Pesticide Residues (JMPR) and the European Community have attempted to rationalise their approach to a grouping of crops/commodities. Most of these groups contain items that are clearly major crop commodities, both in trade and in dietary patterns. Naturally these major commodities are those on which most of the residues trials are carried out. By definition a group MRL applies to all the commodities in the group. When sufficient information is available to estimate the same maximum residues level for most of the major items in a group, it is reasonable to extrapolate this level to cover the other commodities in the group. The general approach of the JMPR to extrapolation has been described (ref.18).

The transfer of data from one situation to another requires knowledge of the factors that the compared situations share with one another, in terms of the pesticide deposit and its disappearance. This requires a detailed knowledge of agricultural practices and growth patterns and characteristics of the crops or varieties. As discussed earlier, meteorological conditions are also of prime importance and it is not valid to extrapolate uncritically between temperate and tropical climates since differences between temperature, humidity and solar radiation can have large effects on the rate and extent of disappearance of deposits.

Extrapolation can be complex and requires considerable knowledge and experience and since there is no definitive scheme for extrapolation, decision makers will often prefer to rely on experimental data, even though the limitations of such data are apparent but not always recognised.

6 CONCLUSIONS AND RECOMMENDATIONS

1. Many of the factors influencing the initial deposit of a pesticide and its subsequent disappearance are not directly controllable and the consideration of pesticide residues and the estimation of maximum levels in crops requires considerable use of skilled estimation and extrapolation.
2. The initial deposit of a pesticide on a crop is the best indicator of the proper application of a pesticide when the edible part of the crop is present and well-developed. The deposit and its distribution influences the average residue at harvest.
3. Studies of available pesticide deposit data indicate that the upper limits and ranges of deposits can be proposed for many crops. These, together with predictions of residues at harvest, provide the framework within which future residues trials could be planned and evaluated.
4. Such trials should focus on factors which govern deposits. The influence of the physical characteristics of the crop and the application equipment which controls spray quality should be studied.
5. The extensive published and unpublished residues data should be used to estimate characteristic distribution patterns for crop/formulation type/method of application, at the time of application and at intervals thereafter.

6. The availability of such patterns would enable Industry and regulatory authorities to -
1. check the proper application of pesticides during residues trials
 2. predict maximum residues levels from relatively few trials
 3. facilitate the use of limited data to establish group MRLs
7. More information should be available on the weight increases in crops during the later stages of growth and on the leaf surface/weight ratios of relevant crops.

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ANNEX. RECOMMENDED APPROACH TO THE EVALUATION OF PESTICIDE RESIDUES IN CROPS

Step 1 Identification and properties of the pesticide.

Requirements : formulation and structure, relevant physical and chemical properties -

- solubility in water
- solubility in organic solvents
- vapour pressure/volatility
- partition coefficient (octanol/water)
- hydrolysis
- oxidation
- photodegradation

Prediction : general behaviour of the compound and its likely stability and reactivity as a chemical in the environment.

Step 2 Formulation and application to the crop - proposed registered uses

Requirements : information on -

- the crop, its physical characteristics and growth stage
- concentration of the product
- concentration of the diluted spray
- rate of application
- numbers and times of applications
- application equipment
- drop spectrum , spray quality
- climatic conditions during application

Prediction : of the initial deposit , both on- and off-target

Step 3. Factors affecting the disappearance(real and apparent) of the deposit

Requirements : information on -

- crop growth after application to assess dilution
- metabolism / degradation in relevant plants
- metabolism / degradation in soil and water
- climatic conditions after application and up to harvest
- identity of metabolites
- systemic/non-systemic activity

Prediction : preliminary estimate of residues at harvest

Step 4. Formal supervised residues trials.

Requirements : trials designed on information from Steps 1 to 3 and executed according to recognised guidelines(ref 18).

Prediction : the results should be used with the preliminary estimate from Step 3 to estimate the maximum residue at harvest for use as an MRL.It may be possible to observe the most frequently found residue.

Step 5. Consideration of extrapolation to other crops.

Requirements : information on the comparative agricultural practices physical characteristics and growth patterns of the crops to be considered, in order to estimate deposits and residues as in Steps 2. and 3. above

Prediction : other crops to which the estimates of the maximum residues levels will apply if required.

Step 6. Prediction of consumer intake - not considered in this report but see IUPAC Report on Pesticides No 22 (ref,20)

Requirements: information on loss/changes in residues at harvest during storage, transport, processing and cooking as relevant.
information on food consumption patterns on a national or regional basis so that the dietary significance of individual food commodities can be estimated.

Prediction : an estimate of the levels of pesticide residues in food as consumed, from which predictions of likely consumer intake can be made.