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OFFICE OF
PREVENTION, PESTICIDES AND
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SUBJECT: Transmittal of Revised Chapter III for March 30 - April 2, 2004 Scientific Advisory Panel Meeting

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Apparently some problems have arisen with the equations in Chapter III of the document, "A Discussion with the FIFRA Scientific Advisory Panel Regarding the Refined (Level II) Terrestrial and Aquatic Models." These problems resulted from the conversion of the file to a PDF format. As a result, we are transmitting hard copies to you.

Please feel free to call on us if you need anything further.

Attachment

cc: E. Fite
I. Sunzenauer

Chapter III. Terrestrial Level II Model

A. Introduction

The major changes, as suggested by the SAP in 2001 (FIFRA Scientific Advisory Panel, 2001), that have been incorporated into the terrestrial Level II model (Terrestrial Investigation Model, TIM), Version 2.0, are:

1. Establishment of generic bird species which represent species occurring in and around agro-environments. The model uses generic attributes to represent the more vulnerable species, yet retains the ability to address specific focal species, when appropriate;

2. Incorporation of a 1-hour exposure time step to allow the inclusion of a bimodal feeding pattern, as well as a higher resolution simulation of daily feeding behavior between treated and untreated areas;

3. Incorporation of an algorithm (Markov Chain) to address serial correlation between sequential foraging events;

4. Development of a new model for estimating pesticide residues in on-field drinking water sources (puddles). This model accounts for a number of parameters affecting puddling after a rainfall event including rainfall amount and duration, soil infiltration rates, evaporation, degradation, and the stochastic nature of field topography and its relation to puddle formation and duration.

In addition to the modifications suggested by the SAP in 2001, an inhalation and dermal model were developed as previously proposed to the SAP in 2000 (FIFRA Scientific Advisory Panel, 2000). As the SAP indicated in their comments in 2001, limited data are available in relation to these routes of exposure and means to estimate effects, resulting in uncertainty in risk estimates. If these routes of exposure are ignored, or are assumed to be minimal, the uncertainty in risk estimates remains unaddressed.

While information is scant on the significance of these routes of exposure for avian species, Driver (1991) showed that dermal and inhalation routes can contribute significantly to the total dose. Furthermore, fundamental exposure principles, especially as related to the relationship between surface area and volume, suggest that the dermal and inhalation routes can contribute significantly to total dose in terrestrial animals.

The uncertainty associated with estimating these routes of exposure is high. However, estimating the contribution of these routes of exposure, even if uncertain, is preferable to making the incorrect assumption that they are minimal in all pesticide use scenarios. The incorporation of the current models for dermal and inhalation exposure provide an important initial step to evaluate the potential significance of these exposure routes to the overall risk estimates, as well as to help

to determine the next appropriate steps.

All of the above risk assessment model modifications resulted in a significant increase in model run-time under the initial software platforms (Excel and Crystal Ball). A change in the computer platforms was made to achieve a more rapid processing time. Version 2.0 of the model was coded using the computer language C and employs Microsoft Excel as the input platform. Using Visual Basic to automate the process, the Excel spreadsheet input data are written to a file that is read by the C code and processed. Selected output data are then written to pre-designed output Excel spreadsheets. As experience is gained, the output can be easily modified to address user needs.

B. General Model Overview

The revised terrestrial Level II model (Version 2.0) is a multimedia exposure/effects model that can be used to address acute mortality levels in generic or specific species over a user-defined exposure window. The spatial scale is at the field level, such that the field and surrounding area are assumed to meet habitat requirements for each species. As an overall simplifying assumption, contamination of edge or adjacent habitat from drift is assumed to be zero. It is anticipated that future modifications to the assessment model will address offsite transport of pesticide residues via drift, though this will require explicit considerations of spatial scale and perhaps more definitive bird behavior data.

The major parameters addressed in the model are:

- Multimedia (vegetation, water, and air) estimates for oral, inhalation, and dermal routes of exposure;
- Food habits of defined generic or selected specific species that are proportioned for each food type consumed by that species;
- Hourly ingestion/inhalation rates of food, water, and air as a function of body weight randomly assigned from specific species or defined generic species body weight distributions;
- Hourly dermal residue transfer rates from contaminated vegetation as a function of body weight randomly assigned from species (generic or specific) body weight distribution and frequency in contaminated areas;
- Frequency of feeding and drinking on the sprayed field, determined in hour time steps
- Distribution of residues on/in vegetation, water (dew and puddles), and air as a function of application rates;
- Degradation/dissipation rates of pesticide residues in each environmental media considered (i.e., food, vegetation, air, and drinking water);
- Acute toxicity dose-response relationship based either on a specific species (when data are available) or inter-species extrapolations from distributions fit to available effects data.

For each individual bird considered in a run of the Level II model, a random selection of

values is made for the major exposure input parameters to estimate an external (ingested) oral dose equivalent for that individual, which accounts for body elimination rates in hourly time steps. The estimated external oral dose equivalent is compared to a randomly assigned tolerance for the individual preselected from the log probit dose/response distribution.

The status of the individual bird (dead or not dead) for this time step is assigned by comparing the estimated oral dose equivalent to the randomly assigned tolerance. If the dose is greater than the tolerance, the individual is scored 'dead' and if the dose is less than or equal to the tolerance, the individual is scored 'not dead'. If scored 'not dead,' the loop is continued until the dose is greater than the tolerance or the user-defined model duration is reached. This procedure is repeated using Monte Carlo sampling and after multiple iterations of individuals, a probability density function of percent mortality is generated. Figure 3-1 provides a simple diagram of the model.

To help ensure that the final model reflects the best available science and that its development is open and clear to the public, the major changes to the model are being presented to the SAP for review and discussion. The following sections discuss the various model modifications and their integration to estimate the magnitude and probability of acute effects to the selected specific/generic species from the exposure to a pesticide. It should be noted that testing (code verification), calibration (adjustments of the model to reflect empirical observations to the extent practical), and sensitivity analysis (ascertaining the out response to changes in input variables) are continuing.

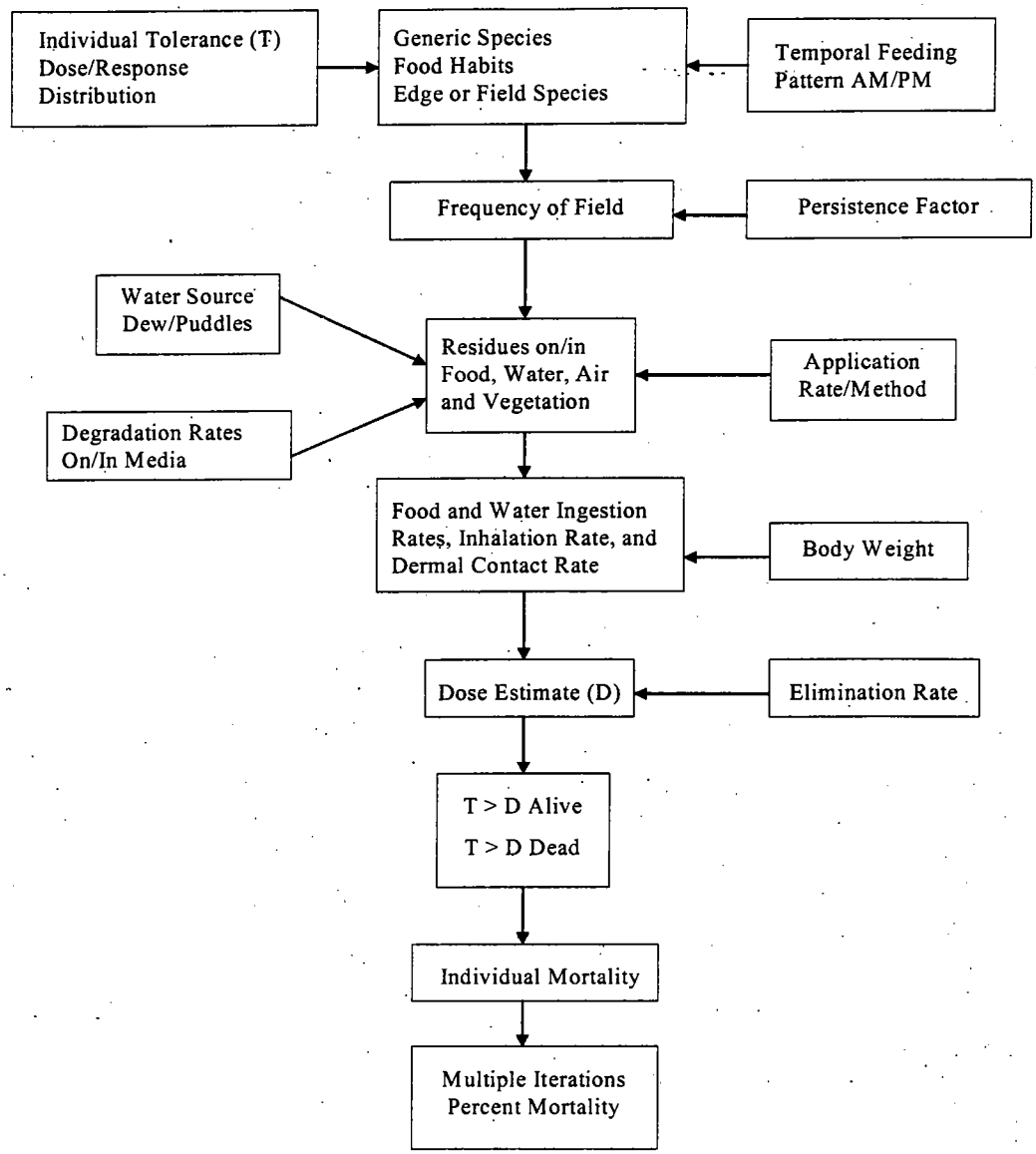


Figure 3-1. Conceptual Model

C. Generic Species

1. Background

Version 1.0 of the Terrestrial model selected a number of actual species (focal species) to represent the large number of potential species of similar biological/behavior characteristics that are found in and around agricultural environments, yet retain some specificity as to the type of organisms using a treated area. The SAP agreed that this approach was reasonable (FIFRA Scientific Advisory Panel, 2001). It was indicated, however, that the adequacy of field data on bird use of a crop is critical to focal species selection. The SAP suggested that using generic species could be simpler and may be less resource-intensive than characterizing a large number of actual species scenarios.

The SAP discussed uncertainties associated with each approach. They indicated that if it can be ensured that the assessment model quantifies the uncertainty in the scenarios and accounts for its effect on the risk estimates, then the scenarios need not be precise and could be based on existing information. They believed that risk estimates based on generic species would have similar high uncertainties due to the variable relationship between exposure factors for generic and actual species. In principle, the SAP indicated, this uncertainty should also be quantified using the same set of data on actual species. If done properly, both approaches would require similar amounts of effort. However, the approach based on actual species has the advantage of risk estimates that are directly relevant to a species known to occur in a given treatment area and do not require further extrapolation from the generic to a known species for site specificity.

As implied in the SAP comments, the key issue in selecting the species lies in the resolution established during the problem formulation step of the risk assessment and the degree to which the risk management decision can tolerate varying levels of uncertainty. The parameters that define a species in relation to risk estimates and contribute to the uncertainty in these estimates in the Version 1.0 model are the species weight and the proportion of food and water consumed from the treated area. In Version 2.0, with the addition of inhalation and dermal exposure, time spent in the treated field becomes an additional parameter. For most species, the uncertainty associated with weight is relatively small and the uncertainty introduced into the assessment due to the absence of data on bird use of crops is substantial. Further complicating an estimate of uncertainty is that, in all probability, the bird use of fields varies greatly from one field to the next in both time and space. Bird use of fields likely depends on numerous poorly quantified variables associated with each field, including the existence and quantity of food and water sources on and off the treated area, adjacent habitats, growth stage of the crop, etc.

Even for the crops and areas where information on bird use has been collected, its applicability to estimating exposure to individuals of a species is highly uncertain. For example, the available census data from various field studies can be used to provide only crude frequency estimates of bird occurrence in crop fields. Frequency information such as this is assumed to reflect bird use of crop areas as a source for food and other resources. The information estimates

of frequency of bird occurrence on treated fields is used to drive the proportion of the diet and drinking water that originates from the pesticide treatment area. The strength of the correlation between frequency on the field and proportion of diet and water consumed from the treated field is unknown. Data on the actual proportions of wildlife daily diet and drinking water obtained from cropped fields would require bird behavior monitoring studies beyond the scope of the current level of assessment refinement.

Given the uncertainty associated with these "frequency on field" estimates and associated extrapolation to exposure estimates, a library of exposure scenarios for specific species within a crop and region, under the current state of knowledge, would provide limited additional understanding of the risks associated with a chemical's use. In some circumstances, and under the current construct of the model, the use of focal species may imply a degree of certainty in the model results that are unfounded. As an interim step between existing risk quotient methods and species-specific analyses, a generic species approach would provide information of the probability and magnitude of effects that could occur. This would advance the risk manager's understanding of the associated risk for the crop/use of interest beyond that provided by risk quotient approaches. This approach would not require the resources to develop specific scenarios for the array of crops where pesticides are used, but for crops where use information has not yet been collected. The problem formulation section of the refined assessment would identify the species occurring in the area of use which the generic species results may represent, and the risk characterization section would discuss the uncertainties in the estimates.

2. Generic Species Approach

The approach proposed for defining the generic species for the Level II model follows the guild method outline by Best et al. (1990), a study that evaluated the propensity of birds to use cornfields in the midwest. In this study, using fixed-width transects, bird numbers and species were counted and recorded as to location in the field (center, perimeter, or edge). All birds observed in and around cornfields were classified on the basis of food type (granivore, insectivore, omnivore, vermivore, frugivore, and carnivore), food substrate (ground/herbaceous, low canopy/shrub, upper canopy/bark, and air), nest substrate (ground/herbaceous, shrub, tree/snag, other), and their occurrence, based on the census data, was categorized as never, rare, occasional, regular, or resident.

Analysis of the data collected indicated that most of the bird species which used corn fields regularly or occasionally are ground-feeding omnivores, whereas the species that rarely or never frequent cornfields are mainly insectivores that forage on woody vegetation. Food substrate preferences were significantly associated with field use. Two bird species that are considered crop field residents were observed to forage on the ground or in low herbaceous vegetation. Seventy-six percent of the species classified as regularly or occasionally using cornfields are also ground feeders. The species that obtain their diet primarily on the bark or in the upper or lower canopy of trees and shrubs were either rarely or never observed in cornfields. Aerial feeders showed no consistent pattern.

Food type was also identified as an important factor which influenced corn field use. Seventy-two percent of the species that regularly or occasionally use cornfields are omnivores, while 70% of the species that either rarely or never use corn fields are insectivores. However, several of the species that do use corn fields are insectivores.

When food type and food substrate are considered collectively, their influence on field use is evident. Ground feeders and low herbaceous feeders comprise all 5 omnivorous species that were crop residents or regular cornfield users and 11 of the 13 species that occasionally used cornfields. Twelve of the 19 insectivores that either never or rarely used corn fields feed either in trees or in shrubs, and an additional 4 of the 19 species are aerial feeders. Thus, 89% (17 of 19) of the omnivores that feed on the ground or in low herbaceous vegetation use corn fields at least occasionally, while 92% (12 of 13) of the insectivores that feed in shrubs or in the canopy or bark of trees either rarely or never were observed in corn fields.

Nest substrate preferences were found to be less important in relation to field use than feeding guilds. However, the resident species with the highest use of cornfields were ground nesters and ground feeders. Species regularly or occasionally using cornfields consisted of a mixture of ground- (5), shrub- (9), and tree-nesting (8) species. In contrast, most (19 of 26) of the birds that rarely or never used cornfields nest mainly in trees or snags.

Because feeding and nesting habits influence habitat use patterns, these attributes were used to define generic species in relation to occurrence on field. Considering variability in residues on different food types, generic species were further defined by dietary preferences as outlined in Table 3-1. Contrary to Best et al. (1990), primary food types were used to classify species in the model. This simply eliminates the need to define the ratios of food types for which limited information is available and highly variable. By assuming obligate feeders, risk estimates should approximate bounds for species with omnivorous food habits of similar food types.

Besides dietary preference in defining a generic species within a guild, three other parameters and associated descriptive statistics are assigned, including body weight, frequency on field, and the on-field persistence factor. The data used to assign values to these variables included the information reported by Best et al. (1990) as well as information on the most common species identified in other field studies (Appendix C). In keeping with a tiered approach, input parameters should be targeted towards defining the more vulnerable species and if additional analysis is deemed necessary, further refinements can be developed. The smallest body sizes and the highest frequency on field are used to define the generic species for each guild. Smaller body size maximizes exposure because food intake, respiration rate, and water requirements are inversely proportional to body weight. High frequency on the field increases the number of time steps where an individual bird is exposed to pesticide residues. For body weight, the smallest average weight of the species in the guild was selected, instead of using a distributional approach that could result in values well outside the observed range, particularly for guilds with few species. For frequency on field, the distribution approach is appropriate and the 95th percentile was selected for this level of assessment. This parameter is highly variable, and therefore the 95th

percentile could occur for a species in the defined guild under some environmental conditions.

The on-field persistence factor is the serial correlation between sequential foraging events. The appropriate on-field persistence factor to apply to these generic species needs further investigation in order to determine the extent to which information is available to parameterize the serial correlation in feeding area selection. However, for initial application of the model, the on-field persistence factor for field resident species is set at 0.8 (i.e., the relatively strong tendency to return to a site to feed that was suggested by the SAP (FIFRA Scientific Advisory Panel, 2001) as an appropriate scenario to model). For edge species, the on-field persistence factor for initial testing is set at 0.6, somewhat lower than field resident species, but still allows for some tendency to return to the same area to feed.

Herbivores are also included in the model. Best et al. (1990) did not report any herbivores associated with corn, and few studies investigating pesticide effects on non-target species have reported herbivores as occurring in study fields. Pesticide incident data, however, from the U.S. Environmental Protection Agency's Ecological Incident Information System, have identified numerous cases involving herbivores, particularly geese and other waterfowl. Moreover, it is reasonable to expect that there are field situations for some otherwise omnivorous species where life stage or seasonal dependance upon vegetation as a food source is high Therefore, for crops that are potential feeding and/or nesting areas for herbivorous avian species, the model includes an option to evaluate this feeding strategy. Body weights for the generic herbivores were selected based on waterfowl species that have demonstrated a preference for terrestrial vegetation as a food source (Canada geese and widgeon). Two weights were selected to address the larger range in sizes of these species with the small species defined as the resident field species, and the larger the edge species. This designation provides some insight into the range of risk for this category of species. Frequency on field and the on-field persistence factor were set equal to the highest weight for the other feeding guilds with the same habitat preference, due to the absence of empirical data for herbivorous species.

It should be noted that information used as the basis for defining the generic species is collected during the early to mid-stages of the growing season (Best et al., 1990). Later in the season, as the height and basal area of the plant canopy increases, the species and feeding guilds of birds that frequent agriculture fields may change. However, the overall effect on the assessment conclusions may not be significant. For example, even if resident ground feeder/nesters are replaced by resident mid-canopy feeder/nesters as the growing season progresses, the defining exposure parameters (body weight and frequency on field) may not be significantly different. Therefore, the generic species selected on the basis of early to mid-stages of the growing season, while somewhat less certain when applied to later stages of the growing season, should still provide reasonable estimates of exposure.

Table 3-1. Generic Species for Level II Assessments

Species	Body Weight (sd) (g)	Frequency on Field (%)	On-field Persistence Factor
Field Resident Insectivore	64.0 (7.0)	98.9	0.8
Field Resident Granivore	19.5 (2.29)	79.3	0.8
Field Resident Herbivore	719 (80.6)	98.9	0.8
Field Edge Insectivore	6.0 (0.13)	66.2	0.6
Field Edge Granivore	12.5 (1.47)	58.7	0.6
Field Edge Herbivore	1264 (29.4)	66.2	0.6

D. Bimodal Feeding Model

The SAP suggested that the 12 hour time steps in Version 1.0 of the model may misrepresent avian activities and thus exposure estimates. It was suggested that allowing more frequent choices for foraging and altering the unimodal feeding pattern to a bimodal feeding pattern would be more representative of avian feeding behavior and may influence exposure estimates. A modeling approach to simulate daily feeding behavior in which each food source is derived in part from treated fields and the balance from untreated areas was proposed. Finally, the assumption of no serial correlation between sequential foraging events was considered unrealistic, especially for territorial species, and would lead to significant under-estimation of risk for a proportion of individuals.

To address these concerns, the model was modified to incorporate a more flexible, probability-based, algorithm of bird feeding behavior. The new algorithm incorporates a bimodal feeding pattern typical of avian morning and afternoon feeding characteristics that are bounded by user-defined morning and afternoon feeding times. Ingestion rates are a function of the duration of the defined foraging period, which can be set to mimic feeding behavior over short or extended periods. The likelihood that not all avian feeding will take place on the treated field is addressed by determining the location (on/off field) of an individual every hour during the feeding period. The hourly location (on/off field) of an individual bird is based on a randomly selected on-field occurrence from a user defined *betapert* distribution. The randomly selected on-field occurrence is used to weight a binomial distribution and is used to predict if an individual is in the treated field for that time step. Location of an individual during non-feeding hours is different for field and edge species. Edge species are assumed to be off field during non-feeding hours. Field species location during non-feeding hours is determined by its initial location in the model run. If on the field in the initial hour, then the individual will be on the treated field during non-feeding hours. If off the treated field in the initial hour, the individual will be off the treated field during non-feeding hours.

To address serial correlation between sequential foraging events, a first-order, two-state Markov chain statistical routine has been incorporated into the model. The tendency to return to a specific area to feed (on-field persistence factor) can be simulated through user-defined probability. The overall average frequency on field is conserved within the specified guild limits. The on-field persistence factor can also be defined to address species with little tendency for repetition of area selection, or for cases where a chemical may reduce the tendency of avian species to return to a specific area to feed or roost. An overview of the modified algorithm is provided below.

1. Modeling Approach

Uptake of pesticide residues depends on the initial concentration of pesticide, pesticide dissipation following application, and how much and when the bird consumes each of the contaminated food sources. In the revised model, exposure time steps begin at midnight of the day of pesticide application. Calculations reflect uptake on an hourly basis, ranging over the analysis interval $0 \le t \le 24D$, where D is the number of user-specified days in the scenario. The time-dependent, hourly pesticide uptake for the kth food source is modeled as:

$$Uptake_k(t_j) = \epsilon_j \times \langle C_k(t_j) \rangle f_k \Delta F(t_j) \frac{Ingestion_k}{BW} \qquad t_j > t_a \tag{3-1}$$

$$Uptake_k(t_j) = 0 \qquad t_j \le t$$

where,

ϵ_j = the on-field presence factor
ϵ_j = 1 if the bird is on the field in the j^{th} hour, ϵ_j = 0 if the bird is off the field in the j^{th} hour
$\langle C_k(t) \rangle$ = the estimated average pesticide residue for the k^{th} food source
f_k = the pesticide treated fraction of the k^{th} food source
$\Delta F(t)$ = the fraction of the total daily intake consumed in the t^{th} hour
Ingestion$_k$ = the daily amount ingested by the bird from the k^{th} pathway
BW = the body weight of the bird
t_a = the hour of the pesticide application.

In the Level II model, total daily ingestion is based on a conventional model of daily metabolic requirement and, for each bird, is allowed to vary slightly from day to day over the analysis period. This means that daily ingestion by pathway will also vary slightly for day to day for a specific bird.

Pesticide residues are modeled as the hourly average residue. The average residue over the j^{th} hour, when the pesticide was applied at $t = t_a$ is

$$\left\langle C_k(t_j)\right\rangle = \frac{1}{(t_j - t_a) - (t_j - t_a - 1)} \int_{tj-ta-1}^{tj-ta} C_k e^{-\lambda_k(\tau - t_a)}\, d\tau = c_k \frac{e^{-\lambda_k(\tau - t_a)}}{\lambda_k}(1 - e^{\lambda_k}) \quad t_j > t_a \tag{3-2}$$

$$\left\langle C_k(t)\right\rangle = 0 \qquad t_j \le t_a$$

where,

λ_k = pesticide dissipation rate on the k^{th} food source, in units of hour^{-1} and where the time t is chosen to take on only integer values.

The revised model is based on the assumption that there are two distinct feeding periods during the day; a morning feeding period and an afternoon feeding period. See Figure 3-2 for an illustration. The beginning and ending times of both the morning and afternoon feeding periods are assumed to vary randomly each day, within specified time windows, and vary from bird to bird. Within the time period marked by the start and end feeding hours, feeding densities are modeled as ***betapert*** distributions (Vose, 1996). The ***betapert*** distribution was selected based on the anticipated state of knowledge at the stage of a Level II analysisrelevant to avian feeding behaviors. The ***betapert*** distribution is useful for modeling situations in which a variable is bounded with known (or estimated) bounds (*min*, *max*) and for which a "most likely value" is known or can be estimated. In this regard, the ***betapert*** is essentially a smoother version of a triangular distribution. See Figure 3-3 for examples of the ***betapert*** density function. More specific and detailed distributions can easily be used as more data become available and as feeding patterns are better characterized.

Like the triangular distribution, the parameters of the ***betapert*** distribution are: a minimum value (*min*), a maximum value (*max*), and a most likely value (*c*). In using a ***betapert*** distribution, one generally works with its beta distribution equivalent in order to utilize readily available numerical routines for calculating the probability density function, cumulative distribution function, and inversion algorithms. The ***betapert***, $\beta_p(min,c,max)$ is related to the standard beta distribution $\beta(\alpha_1,\alpha_2)$ with shape parameters (α_1,α_2) through the following relationships:

$$\beta_p(min,c,max) = min + (max - min) \times \beta(\alpha_1,\alpha_2) \tag{3-3}$$

$$\alpha_1 = \frac{(\mu - min) \times (2c - min - max)}{(c - \mu) \times (max - min)} \qquad \alpha_2 = \frac{\alpha_1(max - \mu)}{\mu - min} \qquad (mean)\,\mu = \frac{min + 4c + max}{6}$$

In terms of equivalent beta densities, the bimodal feeding pattern utilized in the revised model is a composite density comprised of a mixture of two beta probability density functions,

$$f(t) = S \times \beta_P' + (1 - S) \times \beta_P'' \tag{3-4}$$

$$where\ \beta_P' = \beta_p(t; am_{min}, am_{mode}, am_{max}) \qquad \beta_P'' = \beta_p(t; pm_{min}, pm_{mode}, pm_{max})$$

where,

t = the hour of the day
S = the fraction of total daily diet consumed in morning feedings
$(1-S)$ = the fraction of daily diet consumed in afternoon feedings
β_p = the *betapert* density
$(am_{min}, am_{mode}, am_{max})$ and $(pm_{min}, pm_{mode}, pm_{max})$ = the parameters of the commensurate *betapert* densities characterizing the morning and afternoon hourly feeding patterns. (Figure 3-4 illustrates several random bimodal feeding patterns.)

The proportion of diet consumed in a particular hour, $(t,t+1)$, is then

$$(proportion)\Delta F(t_j) = \int_{t_j}^{t_j+1} f(\xi)d\xi = F(t_j + 1) - F(t_j) \tag{3-5}$$

where,

$F(t)$ = the cumulative distribution function for the mixture of *betapert* densities.

The *expected* amount of food consumed in that hour is simply *Ingestion* $\times \Delta F(t)$ where *Ingestion* is the total daily ingestion (grams) for that day. Figure 3-4 illustrates several random feeding patterns based on this bimodal feeding model.

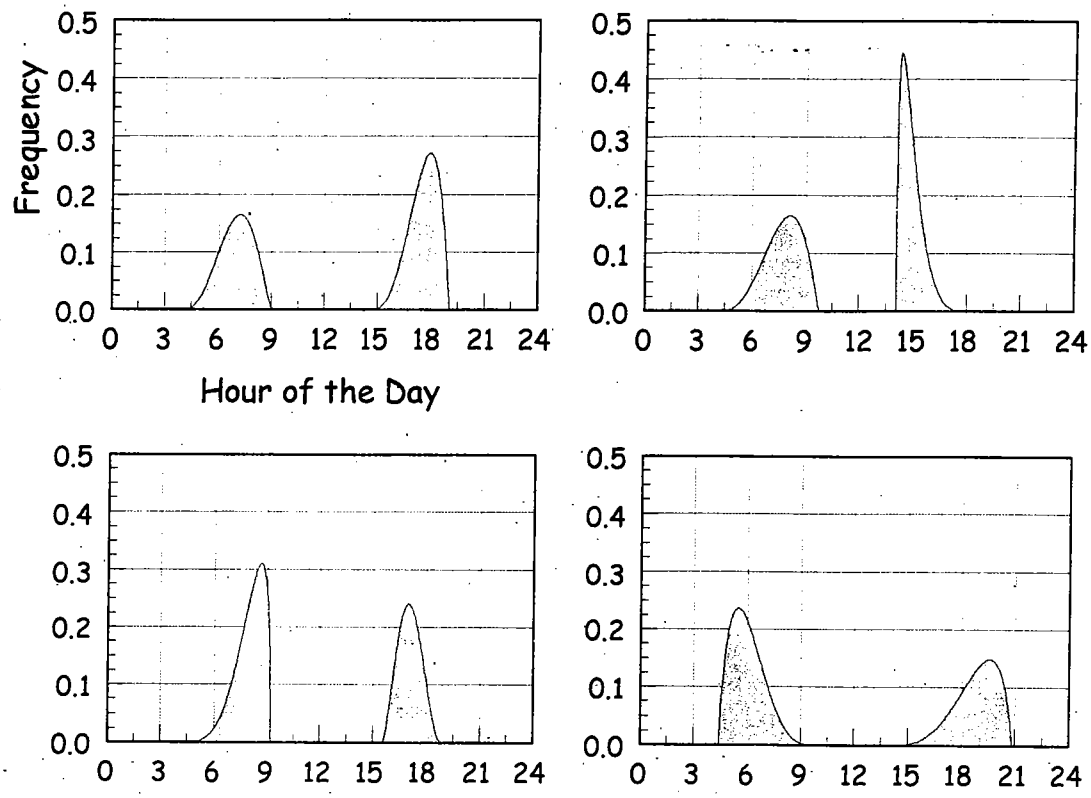


Figure 3-2. Hypothetical examples of the avian bimodal feeding pattern. X-axis is hour of day; Y-axis is daily dietary fraction.

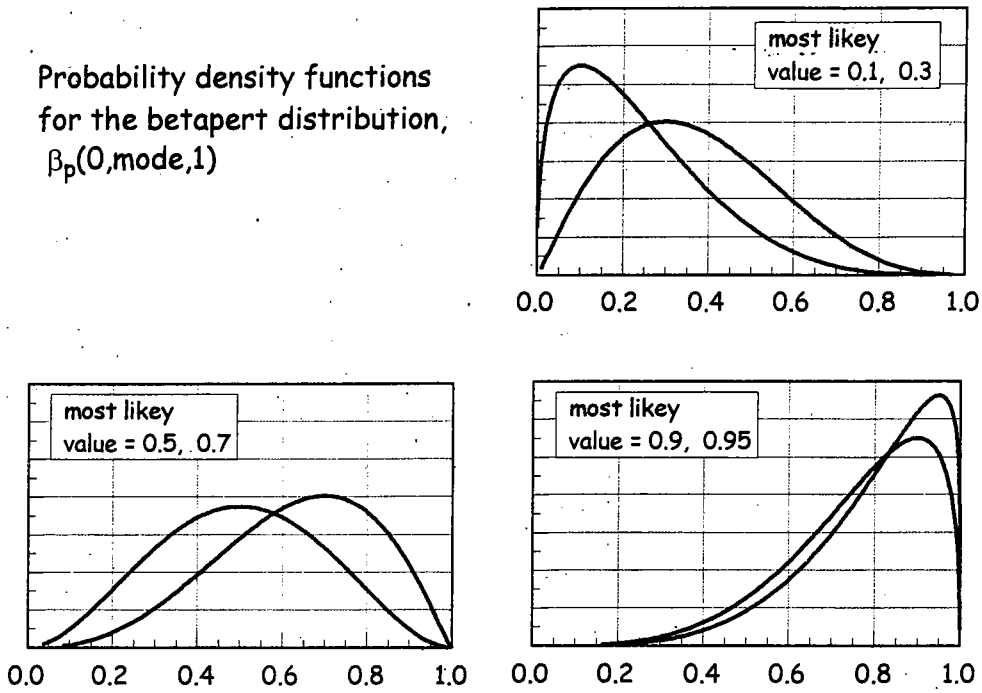


Figure 3-3. Examples of the betapert density used in the bimodal feeding pattern model and the range of shapes that it can assume.

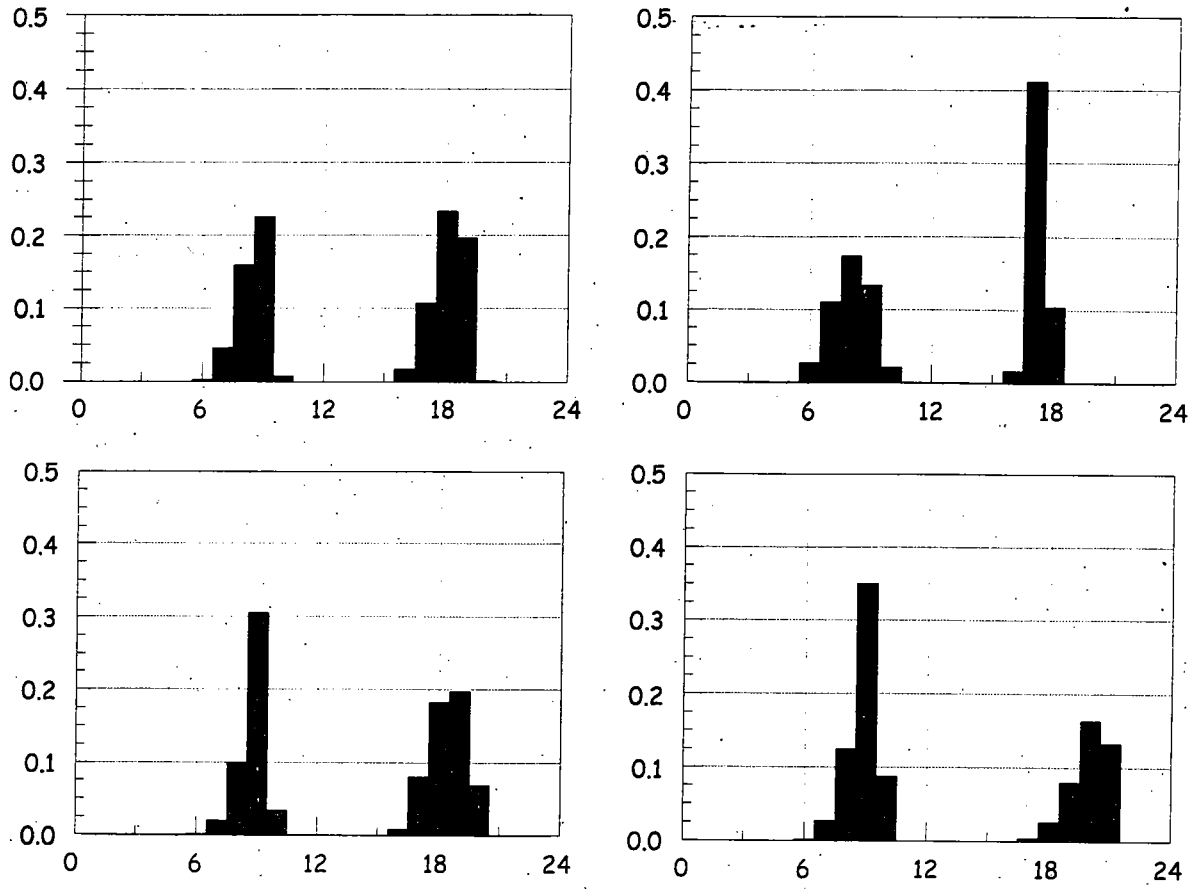


Figure 3-4. Examples of feeding fractions based on bimodal feeding model.

2. Markov Chain Model of On-Field Avian Persistence

In the revised model, ϵ_j, the on-field, off-field behavior parameter, is modeled as a first-order, two-sate Markov chain model. The Markov chain model is a statistical model for the persistence of binary events, in this case, whether or not an individual bird is on or off the field in any particular hour. In this application, two-state refers to the state $X = 0$, the bird is off the field, or state $X = 1$, the bird is on the field. First-order means that the probability of a whether a bird is on the field or off the field in any hour depends only on the state (location) of the bird in the previous hour. A first-order, two-state Markov chain is specified by four transitional probabilities $\{P_{00}, P_{01}, P_{10}, P_{11}\}$ which are conditional probabilities for a bird's state at time t+1 given the bird's state at time t, that is

$P_{00} = \text{Prob}\{X_{t+1} = 0 \mid X_t = 0)$ probability that a bird, now off the field, will remain off the field in the next hour

$P_{01} = \text{Prob}\{X_{t+1} = 1 \mid X_t = 0)$ probability that a bird, now off the field, will be on the field in the next hour

$P_{11} = \text{Prob}\{X_{t+1} = 1 \mid X_t = 1)$ probability that a bird, now on the field, will be on the field in the next hour

$P_{10} = \text{Prob}\{X_{t+1} = 0 \mid X_t = 1)$ probability that a bird, now on the field, will be off the field in the next hour

These transitional probabilities are illustrated in Figure 3-5.

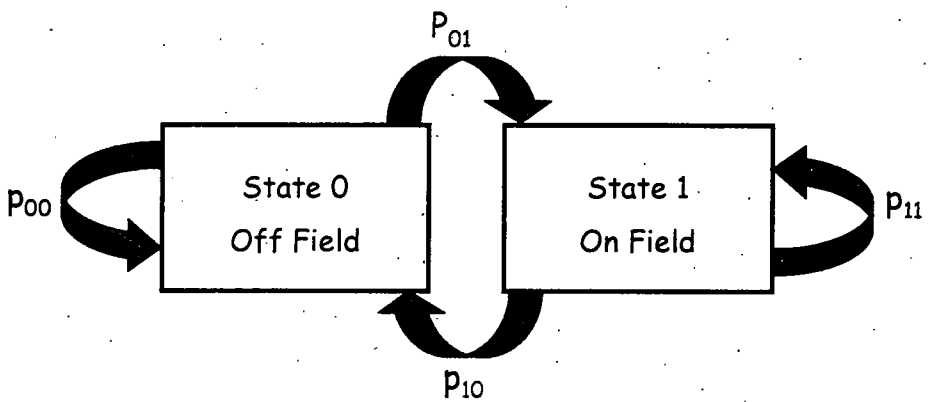


Figure 3-5. The two-state, first-order Markov chain model for avian persistence.

Since the transitional probabilities are conditional, the following relationships hold:

$$P_{00} + P_{01} = 1 \qquad \text{and} \qquad P_{10} + P_{11} = 1$$

The long run probability of a bird being on the field, π_1, is:

$$\pi_1 = \frac{P_{01}}{1 + P_{01} - P_{11}} \tag{3-6}$$

Consequently, the long-run probability of a bird *not* being on the field is $\pi_0 = 1 - \pi_1$. For positive serial correlation, $P_{01} < \pi_1 < P_{11}$ and

$$P_{10} < P_{00} \qquad \text{and} \qquad P_{01} < P_{11}$$

The autocorrelation function for a two-state, first order Markov chain is

$$r_k = (r_1)^k \quad \textit{where } r_1 = P_{11} - P_{01} \tag{3-7}$$

The lag-1 autocorrelation is r_1 and is known as the persistence parameter.

3. Incorporation of the Markov Chain Model into the Level II Algorithm for Avian On-field persistence.

Since $P_{00} = 1 - P_{01}$ and $P_{10} = 1 - P_{11}$, it is sufficient to estimate only one transitional probability in each of this pair of equations to fully characterize the first-order, two-state Markov chain. However, in the revised model, estimates of the distribution of these transitional probabilities are not available. Rather, it is assumed that through field observations, expert judgment, or other means, a screening estimate of the distribution of variability in the long-run, on-field probability, π_1, is available for the relevant bird population, $\pi_1 \sim F(\alpha,\beta)$. A random sample of π_1 represents the long-run, on-field probability for an individual bird. Given an estimate of π_1 for an individual bird, the minimum value the conditional probability P_{11} can assume is:

$$Min of\ P_{11} = Max of \left[\frac{2\pi_1 - 1}{\pi_1}, 0 \right] \tag{3-8}$$

For example, if $\pi_1 = 0.80$, then *Min* of $P_{11} = 0.75$ so that $0.75 \le P_{11} \le 1$. See Figure 3-6.

Let $\Delta P_{11} = 1 - Min\ P_{11}$ be the range of permitted values for P_{11}. Continuing the example

above, $\Delta P_{11} = 0.25$. We assume that the location of the mode of the transitional probability P_{11} be given by:

$$mode\ P_{11} = Min \text{ of } P_{11} + Q \times \Delta P_{11} \qquad 0 \le Q \le 1 \tag{3-9}$$

where Q is a constant to be specified. Q is the fraction of the range of permitted values for P_{11} which helps specify the location of the mode. Figure 3-7 illustrates how Q simply shifts the shape of the distribution of P_{11}. Table 3-2 shows the transitional probabilities for various values of Q and π_1.

In the revised model, P_{11} is treated as a random variable with a triangular distribution

$$P_{11} \sim \text{Triangular}(P_{11}\ Min,\ 1.0,\ P_{11}\ mode).$$

With estimates of π_1, and P_{11}, the remaining transitional probabilities are easily calculated

$$P_{01} = \frac{\pi_1(1 - P_{11})}{1 - \pi_1} \tag{3-10}$$

$$P_{00} = 1 - P_{01} \qquad P_{10} = 1 - P_{11}$$

Figure 3-8 illustrates how avian on-field persistence in the Level II model depends on the long-term, on-field probability π_1 and Q. Figure 3-9 ties the data together by illustrating the interaction of a random realization of the bimodal feeding fraction model with a random on-field sequence based on the Markov chain model to produce a random realization of hourly on-field feeding fractions.

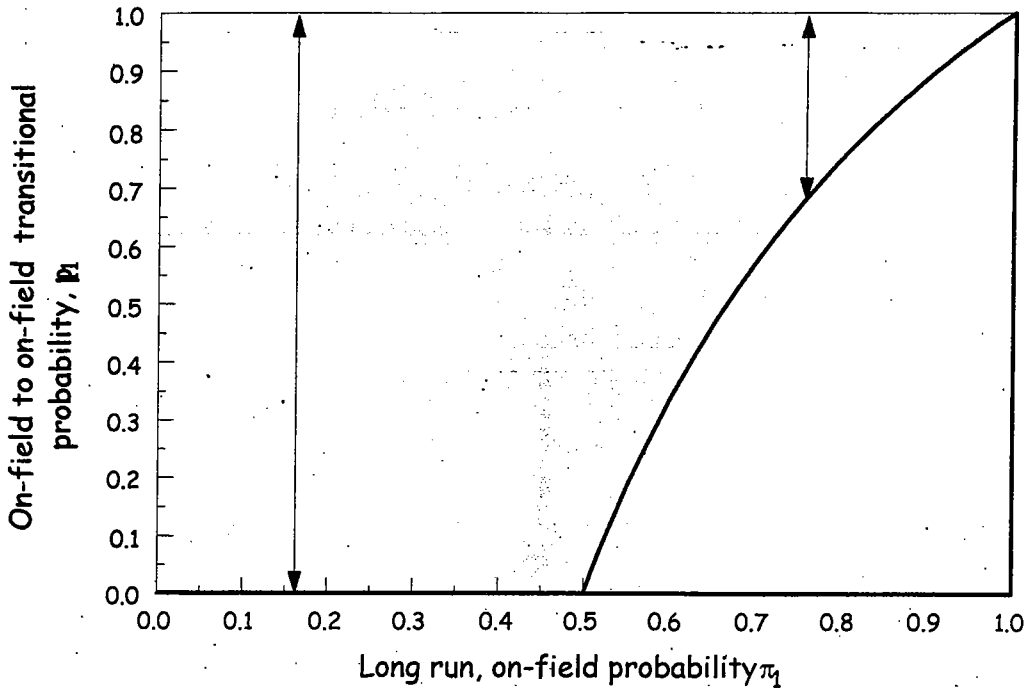


Figure 3-6. Region of valid on-field to on-field transitional probability as a function of long-run, on-field probability, π_1

In this example, $\pi_1 = 0.6$

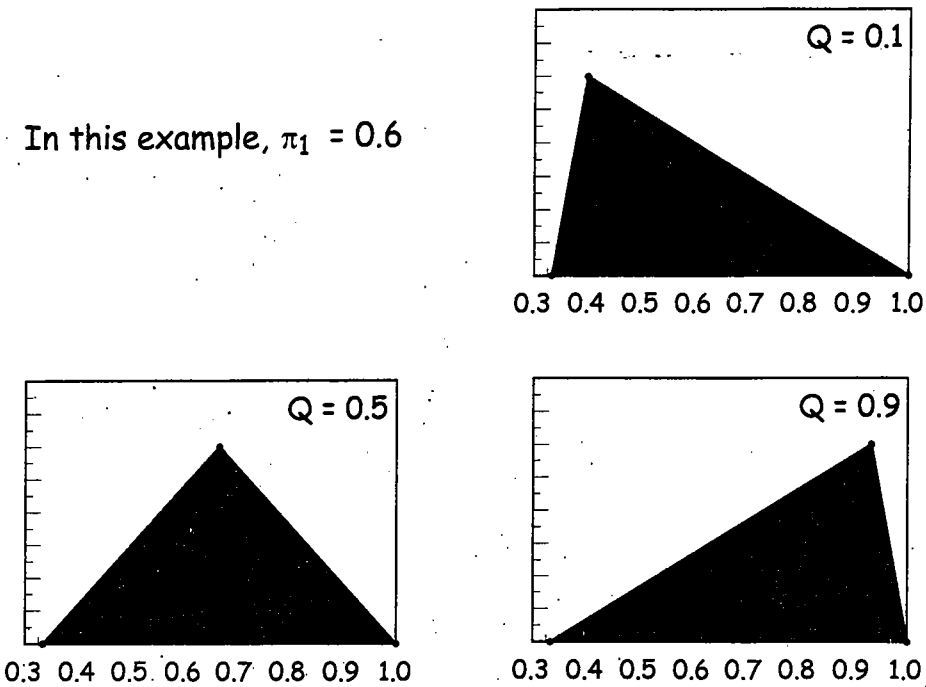


Figure 3-7. Effect of Q on the shape of the triangle distribution of P_{11}.

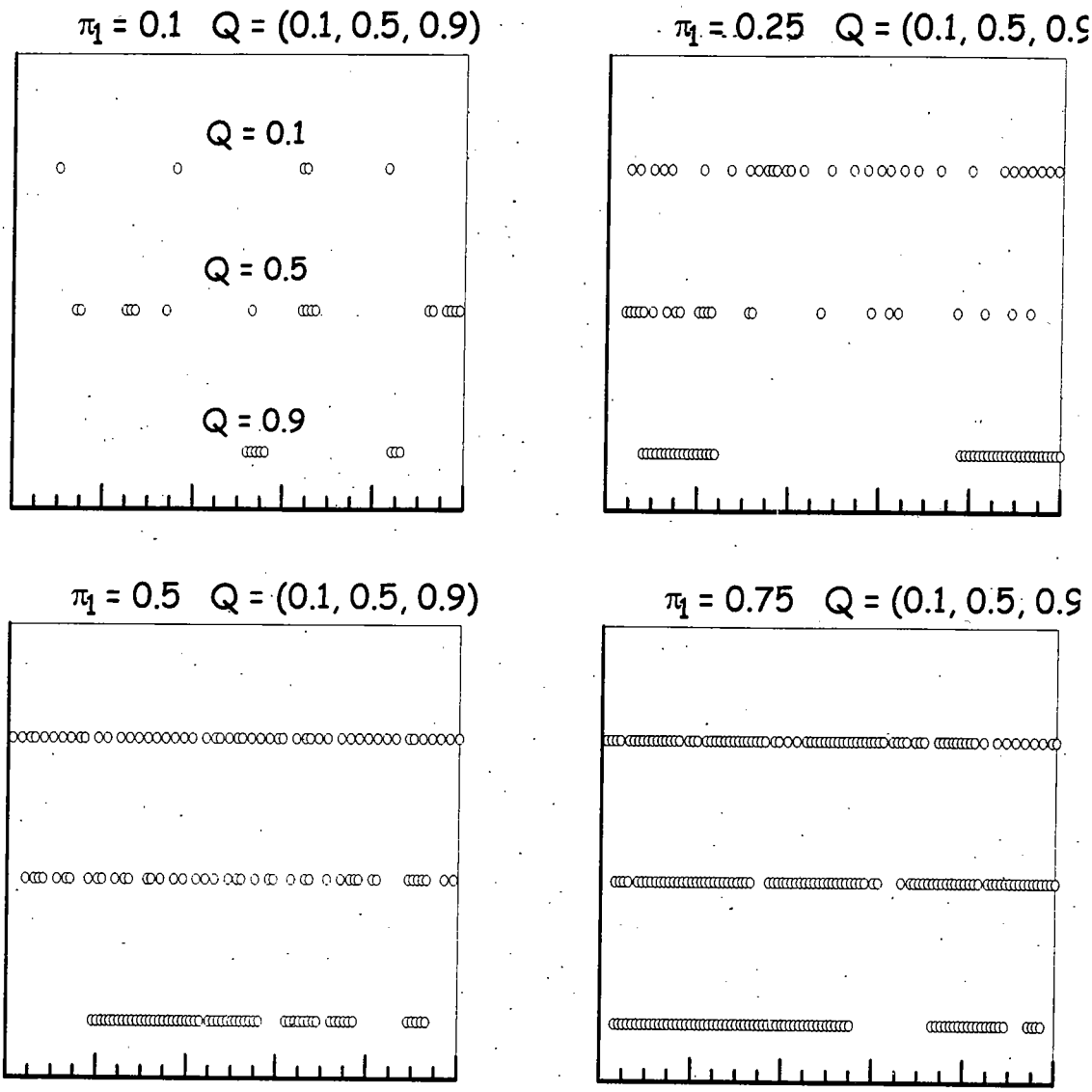
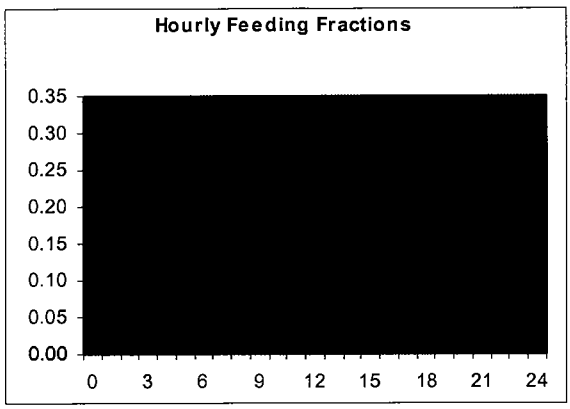
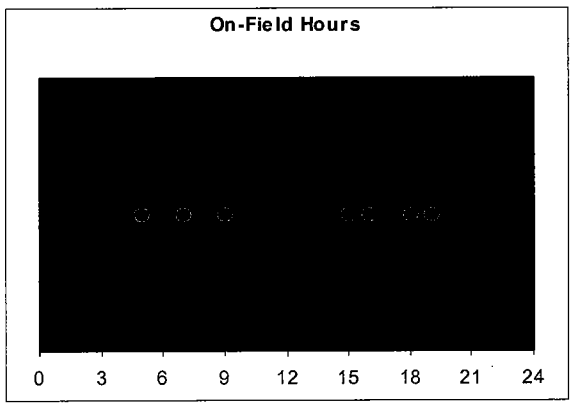


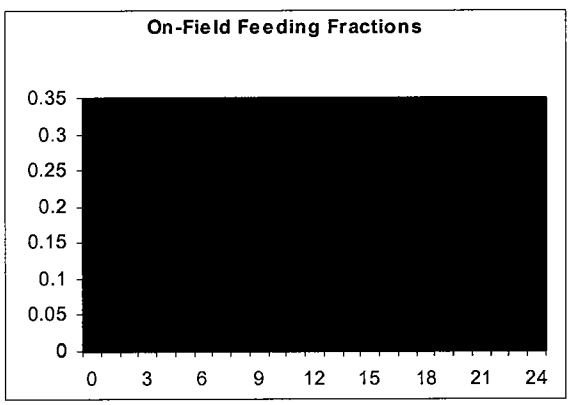
Figure 3-8. Change in avian on-field persistence (persistence) as it depends on long-term on-field probability and on Q. The *x*-axis is 100 time steps (hours). The initial State = 0, bird is off the field. Circles indicate the bird is on the field; blanks mean the bird is off the field. General trends: as π_1 increases, the bird spends more hours on the field; as Q in increases for fixed π_1, the pattern on the field exhibits more consistent runs of consecutive hours on the field.



a). Example of hourly feeding fractions based on bimodal feeding model.



b). Example of on-field hours based first-order, two state Markov chain model.



c). On-field feeding fractions derived by combining Figures (a) and (b) above.

Figure 3-9. Figures (**a**), (**b**), and (**c**) above illustrate the main features of the Level II bimodal feeding model. Only the on-field feeding fractions contribute to ingestion exposures.

Table 3-2. Transition probabilities for various combinations of the long-run, on-field probability, π_1, and Q, the bias factor.

		Π_1 Long-run On-Field Probability				
Q		**0.1**	**0.25**	**0.5**	**0.75**	**0.9**
0.0	**p11**	0.000	0.000	0.000	0.667	0.889
	p01	0.111	0.333	1.000	1.000	1.000
	p00	0.889	0.667	0.000	0.000	0.000
	p10	1.000	1.000	1.000	0.333	0.111
0.1	**p11**	0.100	0.100	0.100	0.700	0.900
	p01	0.100	0.300	0.900	0.900	0.900
	p00	0.900	0.700	0.100	0.100	0.100
	p10	0.900	0.900	0.900	0.300	0.100
0.3	**p11**	0.250	0.250	0.250	0.750	0.917
	p01	0.083	0.250	0.750	0.750	0.750
	p00	0.917	0.750	0.250	0.250	0.250
	p10	0.750	0.750	0.750	0.250	0.083
0.5	**p11**	0.500	0.500	0.500	0.833	0.944
	p01	0.056	0.167	0.500	0.500	0.500
	p00	0.944	0.833	0.500	0.500	0.500
	p10	0.500	0.500	0.500	0.167	0.056
0.8	**p11**	0.750	0.750	0.750	0.917	0.972
	p01	0.028	0.083	0.250	0.250	0.250
	p00	0.972	0.917	0.750	0.750	0.750
	p10	0.250	0.250	0.250	0.083	0.028
0.9	**p11**	0.900	0.900	0.900	0.967	0.989
	p01	0.011	0.033	0.100	0.100	0.100
	p00	0.989	0.967	0.900	0.900	0.900
	p10	0.100	0.100	0.100	0.033	0.011
1.0	**p11**	1.000	1.000	1.000	1.000	1.000
	p01	0.000	0.000	0.000	0.000	0.000
	p00	1.000	1.000	1.000	1.000	1.000
	p10	0.000	0.000	0.000	0.000	0.000

E. Puddle Model

1. Background

The SAP review in 2001 (FIFRA Scientific Advisory Panel, 2001) indicated that the Version 1.0 approach for modeling avian exposure through drinking water seemed reasonable. However, panel members made several suggestions for improving the puddle scenario, including consideration of rainfall amount, rainfall duration, evaporation, soil infiltration rates, plant cover, temperature, chemical partitioning, chemical degradation, and topography.

To incorporate these suggestions, a new puddle model that approximates the most salient processes contributing to pesticide occurrence in puddles on agricultural fields was developed. The model is based on hydrologic balances and mixing-cell approaches. Hydrologic balances are based on area-specific meteorological and soils data and account for the duration and amount of rainfall, evaporation, runoff, and infiltration, while the mixing-cell approach accounts for the chemical fate processes.

2. Model Description

This model is intended to represent the application of a pesticide to an agricultural field and its transport into on-field puddles. Puddles are conceptualized to form in-surface depressions that retain water for periods longer than other areas of the field. Transport of pesticides into the puddles may occur by direct application of the pesticide into the surface depressions or by pesticide runoff from the field. At this time, the model does not consider pesticide transport by soil erosion. During a rain event, the precipitation mixes with a surface layer, and the subsequent pesticide runoff moves into surface depressions, thereby forming puddles. The puddle volume may vary over the duration of a simulation due to infiltration, evaporation, runoff, and puddle overflow. Pesticide mass in the puddles may vary due to runoff input, degradation, and washout. The model can be broken down into four components as described in detail below —1) the field hydrology model; 2) the puddle hydrology model; 3) the field contaminant hydrology model; and 4) the puddle contaminant hydrology model.

a. Field Hydrology

The curve number approach (NRCS, 2003) is used to calculate the quantity of runoff from the agricultural field. For background, Ponce and Hawkins (1996) have provided a timely review of the curve number method and its limitations. The curve number method was chosen for this model because of its simplicity (requiring only one characteristic parameter) and because it is the method used in OPP's pesticide runoff model PRZM (Carsel et al., 1997). With this method, the amount of runoff is related to precipitation as:

$$q_{inches} = \frac{(p_{inches} - 0.2S)^2}{(p_{inches} + 0.8S)} \qquad \text{(for p > 0.2S)} \qquad (3\text{-}11)$$

The maximum retention (S) is determined from the curve number (CN) by

$$S = \frac{1000}{CN} - 10 \tag{3-11}$$

where,

q_{inches} = runoff, [in]
p_{inches} = daily precipitation, [in]
S = maximum retention

This runoff is partially routed into puddles as described in Section 2, Puddle Hydrodynamics. It is also used in the calculations for pesticide transport in Section 3, Field Contaminant Hydrology.

b. Puddle Hydrodynamics

The model considers that an area exists on the agricultural field and produces runoff that enters the puddle ($A_{effective}$), as shown in Figure 3-10. During a storm event, only the precipitation that lands in this effective area and that lands directly in the puddle can contribute to puddle filling. Losses of water from the puddle can occur by infiltration and by evaporation, as well as by overflow. The processes controlling the puddle volume are depicted in Figure 3-11. The puddle volume can increase up to a maximum volume, at which time, overflow occurs. During overflow, the volume remains constant until the inflow is less than the outflow, at which time, volume decreases. The volume of water in the puddle is expressed by:

$$V_{puddle} = V_0 + (Q_{puddle} - EA_{puddle} - IA_{puddle} + PA_{puddle}) \tag{3-13}$$

(for times in which $0 < V_{puddle} < V_{max}$)

and

$$V_{puddle} = V_{max} \quad \text{(for times in which overflow conditions occur)} \tag{3-14}$$

where,

V_{puddle} = water volume of puddle including pore water, [m^3]
V_{max} = maximum puddle volume, [m^3]
V_0 = the volume of water in the puddle at the start of the runoff event, [m^3]
A_{puddle} = area of puddle
E = evaporation rate, [m/s]
I = infiltration rate, [m/s]
P = precipitation rate, [m/s]
Q_{puddle} = runoff flow that enters the puddle, [m^3/s]

The runoff flow rate that enters the puddle (see Figure 3-10) can be calculated from the

runoff depth derived from the curve number method (equations 3-11 and 3-12) along with an estimate of the runoff's duration. As a simplification, the runoff duration is assumed to be equal to the storm duration. The puddle-intercepted runoff is then determined from the following:

$$Q_{puddle} = \frac{(0.0254\,\frac{m}{in})q_{inches}A_{effective}}{T_{storm}} \tag{3-15}$$

where

$A_{effective}$ = field area that contributes runoff to the puddle, [m^2]
T_{storm} = storm duration, [s]

The precipitation rate is determined from the storm volume and storm duration as follows:

$$P = \frac{(0.0254\,\frac{m}{in})p_{inches}}{T_{storm}} \tag{3-16}$$

c. Field Contaminant Hydrology

Contaminant hydrology of the field is addressed by the mixing zone concept, which models the field as a zone of uniform mixing down to a specific depth (Ahuja, 1986; Ahuja and Lehman, 1983; Frere et al. 1980; Haith, 1986; Steenhuis and Walter, 1980). This concept, depicted in Figure 3-12, is analogous to the completely stirred tank reactor (CSTR) concept commonly used in chemical engineering and has been shown to be representative of runoff concentration declines in watersheds (e.g., Hyer et al., 2001; Wallach et al., 1980). Ahuja et al. (1981) showed in ^{32}P laboratory experiments that the completely mixed concept is not entirely realistic and that rainfall mixes with soil in an exponentially decreasing manner with depth. However, Ahuja et al. (1981) did find that an average mixing depth of 0.2 to 0.3 cm could adequately describe ^{32}P transport out of the soil surface. More complex models than the proposed one certainly exist including those involving depth-dependent runoff extraction (Ahuja and Lehman, 1983) and various couplings with vertical transport models (e.g., Mironenko and Pachepsky, 1998; Wallach and van Genuchten, 1990; Wallach et al., 2001). A simple runoff model was selected in order to maintain consistency with other components in the Version 2.0 terrestrial model, and the addition of more complex processes may not be warranted without additional investigation.

Pesticide is applied to the field first. If the pesticide is incorporated into the soil to depths below the mixing zone, then the mass in the mixing zone will be less than the applied mass. For a uniform incorporation, the mass in the mixing zone at the time of pesticide application will be:

$$M_{0,\max} = M_{applied}\left(\frac{h_{mix}}{h_{incorporation}}\right) \quad (3\text{-}17)$$

where,

$M_{applied}$ = the applied mass of pesticide to the field [kg],
$M_{0,mix}$ = the mass of pesticide in the mixing zone at the application time [kg],
$h_{incorporation}$ = depth of pesticide incorporation [m],
h_{mix} = mixing zone depth [m].

After pesticide application to the field, it is assumed to partition according to a linear isotherm as described by:

$$S_{mix} = K_d C_{mix} \quad (3\text{-}18)$$

where K_d is the sorption coefficient [m^3/kg] and degrades due to chemical and biological processes. Water volume in the mixing zone is assumed to not change during the period between pesticide application and the rain event. A mass balance on the mixing zone after application to the field gives:

$$\frac{dM_{mix}}{dt} = (V_{w,mix,0} + m_{mix}K_d)\frac{dC_{mix}}{dt} = -(\mu_a V_{w,mix,0} + \mu_s m_{mix} K_d)C_{mix} \quad (3\text{-}19)$$

where,

M_{mix} = mass of pesticide in the mixing zone
$V_{w,mix,0}$ = initial volume of water in the field mixing zone, [m^3]
m_{mix} = mass of soil solids in mixing zone, [kg]
μ_a = aqueous-phase first-order degradation rate coefficient in mixing zone [s^{-1}]
μ_s = sorbed-phase first-order degradation rate coefficient in mixing zone [s^{-1}]

In practicality, for a pesticide risk assessment, individual sorbed and aqueous rates of degradation are not available for the sorbed and aqueous phases, rather, all that is available is an overall first-order degradation rate derived from laboratory soil/water systems. Because of this data limitation, the pesticide is assumed to degrade independently of any field condition (e.g., soil moisture) up until the rain event occurs by a first-order degradation relationship, and the actual water content in the soil is irrelevant during this time period in the model. This is analogous to the way that OPP currently treats degradation rates in the PRZM model. The overall rate derived from these soil laboratory experiments is equivalent to the following in which the "0" subscript has been dropped from the $V_{w,mix}$ term:

$$\mu_{mix} = \frac{(\mu_a V_{w,mix} + \mu_s m_{mix} K_d)}{(V_{w,mix} + m_{mix} K_d)} \quad (3\text{-}20)$$

where,

μ_{mix} = overall first-order degradation rate coefficient in mixing zone [s^{-1}]

The solution to Equation 3-19 with the initial condition given by Equation 3-17 is:

$$M_{1,mix} = M_{0,mix} e^{-\mu_{mix} t_e} \tag{3-21}$$

where,

$M_{1,mix}$ = mass of pesticide in field mixing zone at start of rain event [kg],
t_e = time to start of rain event [s].

At the start of the runoff event, the mixing zone is assumed to be water saturated. Therefore, the pore water concentration in the mixing zone at the start of the event is:

$$C_1 = \frac{M_{1,mix}}{V_{w,mix} + m_{mix} K_d} \tag{3-22}$$

Runoff is assumed to equilibrate with the mixing zone, so that runoff concentration is equal to the mixing-zone pore-water concentration. Precipitation flow rate is assumed to equal the sum of the runoff and the infiltration flow rates from the mixing zone (i.e., temporal considerations regarding filling the mixing zone are neglected, and we assume that the mixing zone is saturated during runoff). Plant interception of rainfall is also neglected. A mass balance for the field then gives:

$$(V_{w,mix} + m_{mix} K_d) \frac{dC_{mix}}{dt} = - A_{field} P C_{mix} - \mu_{mix} (V_{w,mix} + m_{mix} K_d) C_{mix} \tag{3-23}$$

where,

A_{field} = area of field, [m^2]
C_{mix} = contaminant concentration of water in field mixing zone, [kg/m^3]

Rearranging Equation 3-21 gives

$$\frac{dC_{mix}}{dt} = -\left(\frac{A_{field} P}{V_{w,mix} + m_{mix} K_d} + \mu_{mix} \right) C_{mix} \tag{3-24}$$

or simply as

$$\frac{dC_{mix}}{dt} = -K_{mix}C_{mix} \tag{3-25}$$

where K_{mix} [s^{-1}] is the parenthetical term in Equation 3-22 and represents the effective overall first-order dissipation rate of contaminant in the mixing zone.

The solution to Equation 3-23 with the initial condition given by Equation 3-20 gives the concentration of pore water in the mixing zone (which is equal to the concentration in the runoff) after the rain event begins. The solution is:

$$C_{mix} = C_1 e^{-K_{mix}(t-t_e)} \tag{3-26}$$

In the above mixing-cell model, the volume of water ($V_{w,field}$) and the mass ($m_{s,field}$) of solids in the mixing cell are a function of the assumed mixing-cell depth. By assuming a typical porosity and a bulk density for the field, these parameters are

$$V_{w,mix} = A_{field}h_{mix}\theta \tag{3-27}$$

and

$$m_{s,mix} = A_{field}h_{mix}\rho_b \tag{3-28}$$

where

θ = porosity of the mixing cell region, [unitless]
ρ_b = bulk density of the mixing cell region, [kg/m^3]

d. Puddle Contaminant Hydrodynamics

Initially, a pesticide can exist in surface depressions due to the direct application of the pesticide to the field. It is assumed that a certain depth of soil will equilibrate with the puddle that forms in these depressions, and that below this depth, interactions with the overlying water do not occur. The initial amount of pesticide in the puddle is dependent on the incorporation of the pesticide (as in equation 3-17). The depth of interaction in the puddle is assumed to be the same depth as the field mixing zone; thus the initial mass in the puddle is:

$$M_{0,puddle} = (M_{applied})\left(\frac{A_{puddle}}{A_{field}}\right)\left(\frac{h_{mix}}{h_{incorporation}}\right) \tag{3-29}$$

Degradation in the puddle up until the rain event occurs is assumed to occur as it does on the field:

$$M_{1,puddle} = M_{0,puddle} e^{-\mu_{mix} t_e} \quad (3\text{-}30)$$

As runoff flows across the field, water is routed into surface depressions where it accumulates, forms puddles, and brings additional pesticide into the puddles. Puddle filling may also occur by direct precipitation into the depressions, as described above in Equation 3-13. During the filling process, pesticide mass may be reduced by infiltration and degradation. The pesticide mass balance on these puddles during filling is given by:

$$\frac{dM_{puddle}}{dt} = Q_{puddle} C_{mix} - IA_{puddle} C_{puddle} - V_1 \mu_A C_{puddle} - m_{puddle} \mu_s K_d C_{puddle} \quad (3\text{-}31)$$

where,

M_{puddle} = pesticide mass in puddle, [kg]
Q_{puddle} = runoff flow into puddle, [m^3/s]
I = infiltration rate of puddle, [m/s]
A_{puddle} = puddle area, [m^2]
V_{puddle} = water volume in puddle (including pore water), [m^3]
μ_A = aqueous-phase degradation rate coefficient, [s^{-1}]
μ_S = sorbed-phase degradation rate coefficient, [s^{-1}]
m_{puddle} = mass of solids at equilibrium with puddle, [kg]

During the overflow condition, the volume is held constant, and washout becomes an additional pesticide dissipation process. The net washout flow is:

$$Q_{washout} = Q_{puddle} - IA_{puddle} - EA_{puddle} + PA_{puddle} \quad (3\text{-}32)$$

Under overflow conditions, the pesticide mass in the puddle is described by:

$$\frac{dM_{puddle}}{dt} = Q_{puddle} C_{mix} - IA_{puddle} C_{puddle} - V_{max} \mu_A C_{puddle} - m_{puddle} \mu_s K_d C_{puddle} - Q_{washout} C_{puddle} \quad (3\text{-}33)$$

The pesticide concentration in the puddle is related to the mass under all conditions as follows:

$$C_{puddle} = \frac{M_{puddle}}{\left(V_{puddle} + m_{puddle} K_d\right)} \quad (3\text{-}34)$$

3. Summary of Puddle Model Intervals

There are five distinct intervals in this model which use different model equations to calculate the mass of pesticide in the puddle. With the puddle volume and equation (3-26), the concentration of pesticide in the puddle at any time can be determined. The relevant equations (except for volume calculations) are summarized below.

- **Condition 0. Pesticide applied directly to surface depression (t=0).**

The initial volume of water in the puddle is an input value. For these assessments, the puddle is assumed to be empty. The mass of pesticide in the puddle is:

$$M_{0,puddle} = \left(M_{applied}\right)\left(\frac{A_{puddle}}{A_{field}}\right)\left(\frac{h_{mix}}{h_{incorporation}}\right) \qquad (3\text{-}35)$$

- **Condition 1. Time between pesticide application and rain event ($0 < t < t_e$).**

The volume of water in the puddle does not change between the time of pesticide application and the time of the rain event. The mass of pesticide does change by degradation processes:

$$M_{1,puddle} = M_{0,puddle} e^{-\mu_{aq} t} \qquad (3\text{-}36)$$

- **Condition 2. Rain event and runoff occurring, puddle filling.**

The volume in the puddle changes due to runoff, direct precipitation, evaporation, and infiltration. The mass of pesticide in the puddle is:

$$\frac{dM_{puddle}}{dt} = Q_{puddle} C_1 e^{-K_{field} t} - \left(\frac{\left(V_{puddle}\mu_A + m_{puddle}\mu_s K_d + IA_{puddle}\right)}{\left(V_{puddle} + m_{puddle} K_d\right)}\right) M_{puddle} \qquad (3\text{-}37)$$

We have been unable to find an analytical solution for this equation, so this is solved numerically in the model.

- **Condition 3. Runoff occurring, puddle overflowing.**

The volume in the puddle is constant at V_{max}. The mass of pesticide in the puddle is:

$$\frac{dM_{puddle}}{dt} = Q_{runoff} C_0 e^{-K_{field} t} - \left(\frac{\left(V_{\max} \mu_A + m_{puddle} \mu_s K_d + IA_{puddle} + Q_{washout} \right)}{\left(V_{\max} + m_{puddle} K_d \right)} \right) M_{puddle} \quad (3\text{-}38)$$

The solution is:

$$M_{puddle} = \frac{1}{K_{puddle} + K_{field}} \left[- Q_{runoff} C_{field,0} e^{-K_{field} t} + e^{-K_{puddle} t} \left(Q_{runoff} C_{field,0} + M_{puddle,0} K_{field} + M_{puddle,0} K_{puddle} \right) \right] \quad (3\text{-}39)$$

where

$$M_{puddle} = \frac{1}{K_{puddle} - K_{field}} \left[Q_{puddle} C_{field,0} e^{-K_{field} t} - e^{-K_{puddle} t} \left(Q_{runoff} C_{field,0} + M_{puddle,0} K_{field} - M_{puddle,0} K_{puddle} \right) \right] \quad (3\text{-}40)$$

- **Condition 4. No runoff, rain event passed.**

  The volume in the puddle is decreasing. The mass of pesticide in the puddle is

$$\frac{dM_{puddle}}{dt} = - \left(\frac{\left(V_{puddle} \mu_A + IA_{puddle} + m_{puddle} \mu_s K_d \right)}{V_{puddle} + m_{puddle} K_d} \right) M_{puddle} \quad (3\text{-}41)$$

The solution to equation 3-41 is

$$M_{puddle} = M_{puddle,0} \left(\frac{ft + g}{g} \right)^{\left(\frac{ag - bf}{f^2} \right)} \times \exp \left[- \left(\frac{a}{f} \right) t \right] \quad (3\text{-}42)$$

where
$a = (I+E)\ A_{puddle}\ \mu_a$
$b = V_{pudde,0}\mu_a + IA_{puddle} + mK_d\mu_a$
$f = (I+E)\ A_{puddle}$
$g = V_{puddle,0} + mK_d$

and where all "0" subscripts denote the property's value at the end of the storm.

Note that in practicality, only an overall degradation rate is known (separate sorbed and aqueous phase degradation rates are unknown). In such cases, Equation 3-42 reduces to

$$M_{puddle} = M_{puddle,0} \exp[-\mu t] \qquad (3-42a)$$

where μ is the overall degradation rate.

4. Parameterization

The puddle model requires the input parameters listed in Table 3-3. Some of the parameters are easy to obtain because of their clear physical meaning (e.g., bulk density and porosity). Others, such as mixing cell depth, are purely model approximations of complex physical processes and would require calibration for accurate evaluations. For such cases, literature values can provide useful starting points. Some of these parameters, such as puddle size (W_{puddle}, D_{puddle}) and runoff area fraction (F_{Field}), would vary greatly even at the field scale. For these parameters, the model randomly selects values from assumed distributions. The values given in Table 3-3, are suggested as initial starting points for use in model evaluation. As more data are obtained and as model testing proceeds, the values will be appropriately adjusted.

The mass applied ($M_{applied}$) is determined from the required pesticide application rate. The mixing zone depth parameter (h_{mix}) is critical, sensitive, and difficult to estimate. Some values for h_{mix}, taken from the literature, are summarized in Table 3-4. For initial testing, an h_{mix} value of 0.1 cm is used because it is in the range of values listed in Table 3-4 and has some experimental backing. Values for bulk density, porosity, and curve number will be based on current guidance for developing PRZM scenarios (USEPA, 2002). Precipitation amount (p_{inches}), rainfall duration (T_{storm}), and evaporation rate (E) will be based on the meteorological data used in PRZM/EXAMS standard scenarios. Puddle runoff area is based on a conceptualization due to the absence of empirical data and is randomly generated to account for expected variability. The minimum and maximum run-off areas were based on the concept of a field depression in the center of a circle varying in radius from 10 to 50 meters with a mode of 20 meters. The resultant fractions of the 100 m by 100 m area of the field for run off are 0.03, 0.12, and 0.78 for the minimum, mode, and maximum, respectively, and a betapert distribution was assumed. The two degradation parameters, μ_a and μ_s, are taken from studies submitted for pesticide registration. In most cases, only the overall degradation rate will be known from such studies, and in these cases, μ_a will be set equal to μ_s. The average infiltration rate (I_a) is estimated from the implied rate from the curve number and is assumed to be a uniform distribution with a minimum value of 20 percent and a maximum of 1.20 percent of the average infiltration rate. These values are based on the perception that the formation of puddles may result from surface depressions being formed due to compaction and, thus, infiltration rates would vary in a manner less than general field infiltration rates. For the initial volume of water (V_0), the puddle is assumed to be initially dry. The maximum puddle volume is entered as a betapert distribution with minimum dimension of 0.15 m long x 0.15 m wide x 0.02 m deep, maximum dimensions of 3.0 m long x 3.0 m wide x 0.15 m deep and mode dimensions of 1.0 m long x 1.0 m wide x 0.089 m deep. These dimensions are

based on the best professional judgement, due to the absence of empirical data on puddle size. The mass of solids associated with the puddle (m_{puddle}) is another parameter that is difficult to estimate and indicates how much of the soil at the bottom of the puddle can be assumed to be at equilibrium with the water in the puddle. As a first estimate, we assume that it is the same as the field mixing zone depth (h_{mix}).

Table 3-3. List of input parameters for puddle model.

Parameter	Units	Description	Recommended Value
$M_{applied}$	kg	Amount of pesticide applied to field	From pesticide label
A_{field}	m^2	Max Runoff Area	10,000
F_{field}		Runoff Fraction of A_{field} for a puddle	Monte Carlo Betapert Distribution[(a)] min=0.03, max=0.78, mode=0.12
h_{mix}	m	depth of field mixing zone	1 cm (Steenhuis and Walter, 1980)
θ	--	porosity of mixing zone	0.5 typical
ρ_b	kg	bulk density of mixing zone	1500 kg/m^3 typical
CN	--	Curve number	User input based on PREZM/EXAM Standard Scenarios
p_{inches}	inch	Precipitation	NOAA meteorological data
T_{storm}	s	Duration of rain event	NOAA meteorological data
W_{puddle}	m	Width of puddle	Monte Carlo Betapert Distribution[(a)] min=0.15, max=3.0, mode=1.0
μ_a	s^{-1}	First-order aqueous-phase degradation rate coefficient	Product chemistry
μ_s	s^{-1}	First-order sorbed-phase degradation rate coefficient	assume the same as aqueous degradation
E	m/s	Evaporation rate	NOAA meteorological data
I	m/s	Infiltration rate in puddle	Monte Carlo Uniform Distribution[(a)] min=0.2((total rainfall –total runoff)/T_{storm}), max=1.2((total rainfall-total runoff)/T_{storm}), set from implied infiltration rate for the curve number
V_0	m^3	Initial water content in puddle	0
D_{puddle}	m	Depth of puddle	Monte Carlo Beta Distribution[(a)] min=0.02, max=0.15,mode=.089
V_{max}	m^3	Maximum water content of puddle	D_{puddle} x W_{puddle} x W_{puddle}
m_{puddle}	kg	Mass of solids associated with puddle	assume a 1 cm interaction, same as h_{mix}, and bulk density is same as ρ_b

[(a)]Assumed distribution based on best professional judgment.

Table 3-4. A Summary of Mixing Zone Depths from the Literature

Mixing Zone Depth (cm)	References	Notes
1	Frere et al. (1980)	CREAMS model
1	Carsel et al. (1984)	PRZM 2*
0.2–0.6	Donigan et al. (1977)	ARM model
>0.2–0.4	Zhang et al. (1997), (1999)	Satisfactory for well drained soil
1	Steenhuis and Walter (1980)	From review of references therein
1	Haith (1980), (1986)	Assumed (uncalibrated)
0.9	Snyder and Woolhiser (1985)	Flume study
0.2–0.3	Ahuja et al. (1981)	Average experimental effective depth lab-size plot
0.2	Ahuja (1982)	
0.5–1	Havis et al. (1992)	Laboratory and intermediate scale field experiment (260 m^2)

*PRZM has since been modified and is now without a complete mixing cell approach (Carsel et al., 1997).

5. Future Developments

Model outputs need to be compared to field data so that parameters can be adjusted appropriately. An example of parameter estimates that could be improved include the depth of solids interaction in the puddle and the field mixing depth, both of which are difficult to measure and are primarily fitting parameters with less physical meaning than the other parameters. Other needed improvements in model inputs include the puddle size parameters, which were selected using professional judgement without the assistance of any actual data. A scientific analysis of puddle dimensions may be useful to improve these parameter values.

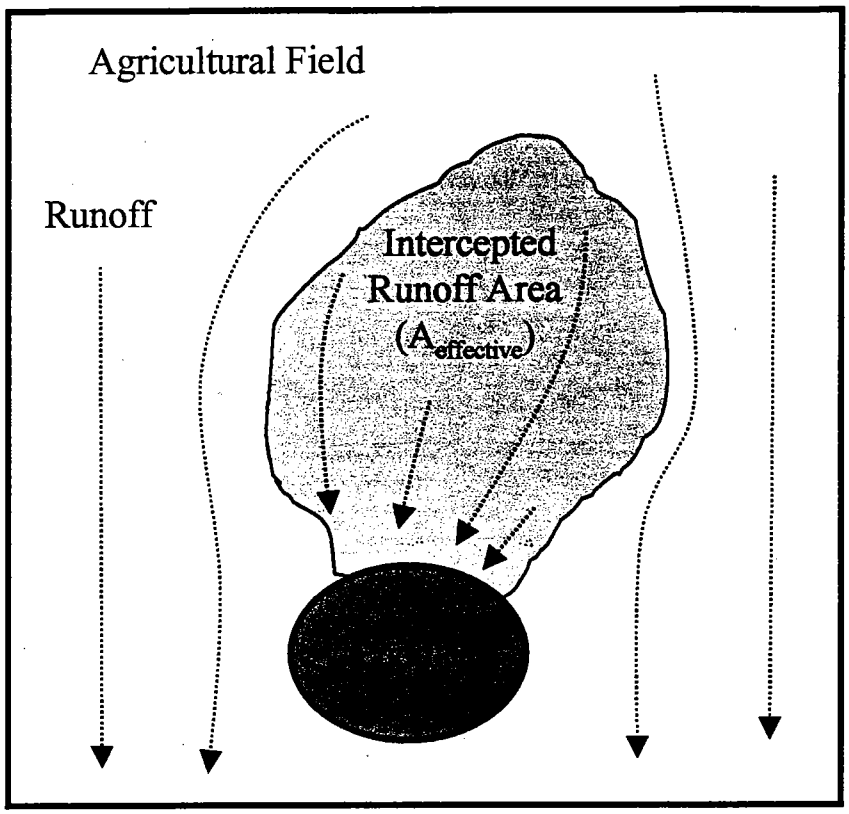


Figure 3-10. Depiction of the area that contributes to runoff to the puddle.

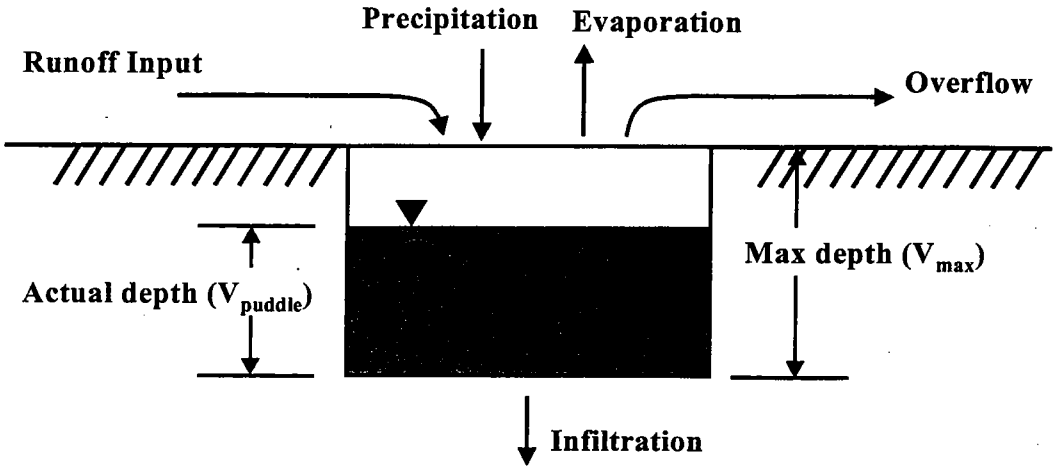


Figure 3-11. Depiction of the hydrologic processes controlling puddle volume variation.

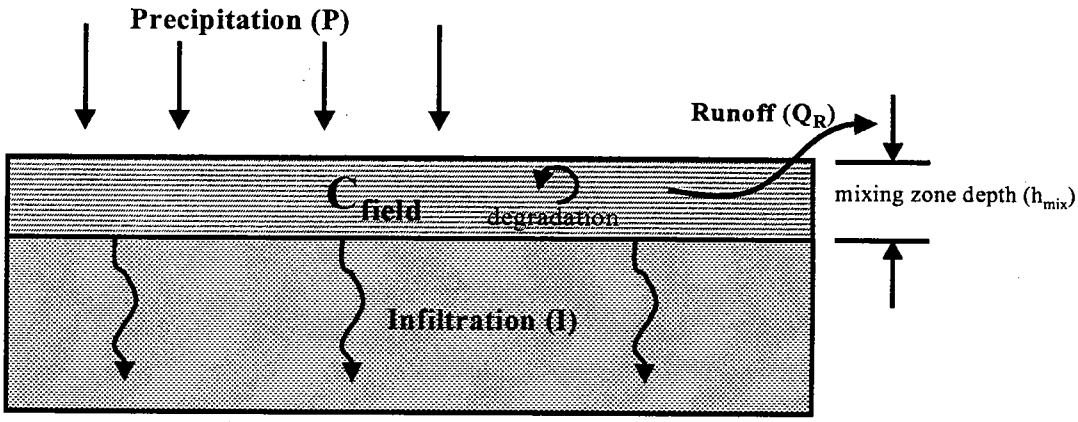


Figure 3-12. Depiction of the field mixing zone concept.

F. Model for Inhalation Exposure

Existing assessment methods for pesticide risks to avian wildlife do not consider the potential for exposure via inhalation. The work of Driver et al. (1991) suggests that inhalation of pesticides may, in some circumstances, contribute significantly to acute pesticide risks to birds. Furthermore, lines of evidence from underlying principles of toxicokinetics as related to surface area to volume ratios suggest that the dermal and inhalation routes can contribute significantly to total dose in terrestrial animals. Existing assessment methods do not include a quantitative evaluation of the potential for pesticide inhalation and assume that avian wildlife risks from inhalation of pesticides are inconsequential.

There are a number of challenging opportunities to incorporate a consideration of the inhalation route in avian pesticide risk assessments. These include 1) development of an assessment method that can be based on existing environmental fate and effects testing, 2) prediction of air concentrations near ground and near field, and 3) relating pesticide exposure via the inhalation route to toxicity data generated through oral exposure testing methods. These challenges can be effectively met through the consideration and incorporation of existing Agency methods in other programs estimating inhalation exposure, effects, and risk.

1. General Inhalation Exposure Model

The general inhalation exposure model considers two inhalation pathways. These are the direct inhalation of airborne droplets immediately following pesticide application, and inhalation of vapor phase pesticide. Inhalation of particulate associated pesticide with fugitive dust emissions is not currently incorporated in the model, but could be incorporated in subsequent versions.

For both inhalation routes currently modeled, the exposure is expressed on inhaled dose (mass of pesticide inhaled over a given time period) rather than an absorbed dose (mass of inhaled pesticide absorbed across the respiratory membrane). The mathematical representations of the models are as follows:

Respirable Droplet Inhalation

$$DID(mg/kg)=\frac{(A_{rate})(1/RH(F_{respired})(V_{inhalation})}{(1000)(BW)} \qquad (3\text{-}43)$$

where:

DID = Droplet Inhalation Dose mg/kg

A_{rate} = application rate from label converted to mg/m^2

RH = height of spray release (m), user defined (defaults are 1 m for ground spray and 3 m for aerial application)

$F_{respired}$ = volumetric droplet spectrum segregated by upper size limit of

respired particles for birds (See section on $F_{respired}$ for further information)
$V_{inhalation}$ = inhalation volume (L) (See section on $V_{inhalation}$ for further information)
1000 = units conversion m^3 to L
BW = bird weight (kg)

Inhalation of Vapor Phase Pesticide

$$VID(mg/kg) = \frac{C_{air} V_{inhalation}}{BW} \quad (3\text{-}44)$$

where:

VID = Vapor inhalation dose mg/kg
C_{air} = concentration of the pesticide in air at time t (mg/L) (See section on C_{air} for further information)
$V_{inhalation}$ = inhalation volume (L) (See section on $V_{inhalation}$ for further information)
BW = bird weight (kg)

$F_{respired}$ Fraction of Spray Droplets Respired

The inhalation exposure model for airborne pesticide application droplet considers exposure only to those droplets that may enter the avian lung. It is expected that there is an upper bound particle size that may enter this area of the respiratory tract, which is termed the respirable particle size. Appendix D provides an upper bound estimate of 7 μm. The fraction of applied pesticide spray is therefore assumed to be the fraction of the spray droplet spectrum that falls at or below this diameter. Spray droplet spectra for a given application scenario are derived from AgDrift model outputs for given spray nozzle types, application equipment, and application conditions.

$V_{inhalation}$ Inhaled Air Volume

In any given exposure time step within the model where inhalation exposure is calculated, a volume of inhaled air is determined as follows:

$$V_{inhalation} = R_{rate} \times ED \quad (3\text{-}45)$$

where,

R_{rate} = respiration rate (l/min),
ED = Exposure duration (min),

where respiration rate is an allometric relationship relating avian resting respiration rate to body weight. This value is multiplied by 3 to approximate a field respiration rate (USEPA, 1993):

$$R_{rate} = \frac{(284 BW^{0.77}) \times 3}{1000} \tag{3-46}$$

Duration of exposure is sixty minutes for inhalation modeling and is consistent with the overall model time step duration.

2. Consideration of Other Agency Approaches in Modeling the Air Concentration

US EPA's Office of Solid Waste Hazardous Waste Identification Rule (HWIR) Farm Foodchain Model (USEPA, 1999) includes a model to estimate plant concentrations from vapor phase concentrations of contaminants. This model calculates plant concentrations as a result of wet and dry deposition routes and presents a mathematical solution for deposition of organics with octanol/water partition coefficients below log K_{ow} 5 that account for both wet and dry deposition. The model also presents a mathematical solution of high octanol/water partition coefficient chemicals (log K_{ow}>5) in which plant concentration estimates do not consider wet deposition, but are derived from a two-compartment equilibrium relationship. This later approach, though simple, is useful as a basis for modeling air concentrations in low-mixing zones within a crop canopy.

The HWIR Food Chain model is as follows:

$$PV = \frac{(Cv_{ave})(Bv)(Vg_{ag})}{1000 \rho_{air}} \tag{3-47}$$

where,

PV = plant concentration due to vapor (mg/kg DW)
Cv_{Ave} = the vapor phase concentration of chemical in air (μg/m^3)
Bv = the air-to-plant biotransfer factor ([μg/g DW]/[μg/g air])
Vg_{ag} = an empirical correction factor (unitless)
1000 = a units conversion factor (g/m^3)
ρ_{air} = the density of air (constant at 1.19 g/L)

$$Bv = \frac{\left(\rho_{air} B_{vol} / 9\right)\left(\left(100 - MAF_{leaf}\right) / 100\right)\rho_{leaf}}{Bv_{ecf}} \tag{3-48}$$

where,

Bv = the air-to-plant biotransfer factor ([μg/g DW]/[ug/g air])

ρ_{air} = the density of air (constant at 1.19 g/L)
$B_{vo}l$ = the biotransfer factor ((µg/L freshweight leaf)/µg/L air)
MAF_{leaf} = the moisture content in leaf (%)
ρ_{leaf} = the density of the leaf (g/L fw)
Bv_{ecf} = the empirical correction factor for Bv (unitless)

$$\log B_{vol} = 1.065(\log K_{ow}) - \log(H/RT) - 1.654 \quad (3\text{-}49)$$

where,

B_{vol} = the biotransfer factor ((µg/L freshweight leaf)/ug/L air)
K_{ow} = octanol/water partition coefficient
H = Henry's Law constant (atm/m^3/mol)
R = the universal gas constant (8.205E-05 atm/m^3/mol-K)
T = air temperature (constant at 298.1 K)

The HWIR model assumes the following values, which are incorporated into the pesticide inhalation model:

MAF_{leaf} - HWIR model provides central tendency numbers for forage, leaves, fruit, etc., with a leaf value of 85%

ρ_{leaf} - HWIR model assumes 770 g/L

Bv_{ecf} - HWIR model uses an empirical correction factor for BV of 100

Vg_{ag} - HWIR model uses a factor of 0.01

In order to solve for the vapor phase concentration in air, a rearranged set of equations from the HWIR model could be used directly in a model to obtain a prediction of air concentrations at a given point in time from known plant pesticide residues. However, it should be noted that the HWIR model is based on an assumption of a continuous influx of chemical in a vapor state from a known source (i.e., there is no mass limitation for the modeled contaminant). This results in little need to account for total mass of the available chemical once an equilibrium is achieved. In contrast, a pesticide application involves a finite mass of pesticide; consequently, any equilibrium model must consider the available chemical mass and construct a predictive air concentration model that avoids estimations of air concentrations which exceed the total mass of pesticide available from source plant material over time.

3. Combining the HWIR Approach with Mass Conservation in a Two-Compartment Equilibrium Model

The problem of mass conservation has been addressed in a two-compartment equilibrium models used to estimate pesticide concentration in water and sediment in rice paddy environments. The rice paddy model estimates soil and water concentrations as a function of total mass applied to the paddy and subsequent partitioning of that mass between sediment and overlying water.

The rice paddy model is as follows:

$$W_{con} = \frac{10^9 M_T}{V_T + m_{sed} K_d} \tag{3-50}$$

where,

M_T = the total mass of pesticide in kg applied to 1 ha of paddy

V_T = 1.016 x10^6 L the volume of water in a paddy 1 ha in size, 4 inches (10.16 cm) deep

m_{sed}, = the mass of sediment, 130,000 kg, in the 1 ha paddy in the top 1 cm interaction zone (sediment bulk density was assumed to be 1.3 kg L^{-1}).

10^9 converts the units for mass from kg to μg.

K_d = the sediment:water partition coefficient

A similar two-compartment model has been employed in the revised avian risk assessment model to predict air concentrations in treated agricultural fields. Plant residues for the pesticide (based on the existing estimates used for dietary exposure elsewhere in the terrestrial model), combined with assumption of standing crop per unit area, are used to estimate the total mass of pesticide available for partitioning between crop leaf and canopy air. The air compartment is set to 1 ha area, with a height set at the top of the canopy at time of application. The available pesticide residue is then partitioned between the two compartments thought the application of the volume-based biotransfer factor B_{vol} developed for the HWIR model. The total available residues establishes an upper limit of available pesticide mass.

$$C_{air} = \frac{C_{plant} m_{plant}}{V_{air}(1000) + \left(m_{plant} \left(B_{vol} / \rho_{plant} \right) \right)} \tag{3-51}$$

where,

C_{air} = concentration in air mg/L

C_{plant} = the pesticide residue in plants (mg/kg fresh weight) linked to dietary exposure model predictions for foliar concentrations

m_{plant} = the mass of plant per hectare (kg/ha)

V_{air} = the volume of air in 1 ha to a height equal to the height of the crop canopy (m^3)

1000 = units conversion m^3 to L

B_{vol} = the volume-based biotransfer factor ((ug/L freshweight leaf)/ug/L air) as calculated by the HWIR model (log B_{vol} = 1.065 log K_{ow} - log(H/RT) -1.654)

ρ_{plant} = the density of the crop tissue assumed as fresh leaf kg/L (use 0.77 as per HWIR model)

Table 3-5. Inhalation model parameters.

Parameter	Units	Description	Recommended Value
A_{rate}	mg/m^2	labeled rate of pesticide a.i. application	User defined
RH (release height)	m	height of pesticide release	User defined Defaults: 3 - aerial applied 1 - ground applied
$F_{respired}$	unitless	fraction of applied pesticide as respirable droplets	User defined from AgDrift droplet spectra and upper bound 7 um droplet diameter
$V_{inhalation}$	L	volume of inhaled air over time step	respiration rate * duration of exposure
R_{rate} (respiration rate)	L/min	field respiration rate	$\text{rate} = \frac{(284*\text{bodyweight(kg)}^{0.77})*3)}{1{,}000}$ (USEPA, 1993)
ED (duration of exposure)	min	duration of inhalation exposure for a time step	60 for vapor phase exposure User defined for droplet inhalation exposure
body weight	kg	bird body weight	see text on generic bird types
C_{air}	mg/L	vapor phase pesticide concentration in air within the plant canopy	$\frac{C_{plant} * m_{plant}}{V_{air}(1{,}000)+(m_{plant}*B_{vol}/\rho_{plant})}$
C_{plant}	mg/kg	pesticide concentration in foliage	based on dietary residue distributions
m_{plant}	kg	mass of crop on 1 ha at application time	user defined
V_{air}	m^3	volume of air above a 1 ha field to the height of the canopy at application time	V_{air} = canopy height * 10,000
canopy height	m	height of crop canopy at pesticide application	user defined

B_{vol}	(ug/L fw leaf)/(ug/L air)	B_{vol} is the volume-based biotransfer factor	log B_{vol} = 1.065 log K_{ow} - log(H/RT) - 1.654
K_{ow}		octanol/water partition coefficient	user defined
H	atm/m^3/mol	Henry's Law constant	user defined
R	atm/m^3/mol-K	universal gas constant	8.205E-05
T	°K	air temperature	298.1
ρ_{plant}	kg/L	density of the crop tissue assumed as fresh leaf	0.77 as per HWIR (USEPA, 1999)

5. Scenarios for Consideration of Pesticide Exposure Through Inhalation

Exposure through inhalation from applied pesticide droplets is considered only for the first exposure time step immediately following the pesticide application. It is assumed that a suspended droplet will have either settled or cleared from the application area by the next time step, 60 minutes after application. Inhalation exposure for vapor phase pesticide is calculated for every time step of the model run, in which the individual bird is predicted to be present on the treated area. For edge residents, vapor-phase inhalation exposure is estimated for all time steps in which the bird is actively feeding in the treated area. For in-field residents, vapor phase inhalation exposure is estimated for all time steps in which the bird is actively feeding in the treated area as well as all non-feeding periods where the bird has returned to the field for periods of inactivity. Version 2.0 of the model does not reduce the respiration rate of non-active birds; this remains an option for subsequent model versions.

6. Relating External Inhalation Dose to Oral Dose Equivalents

Currently, the Agency does not have a data requirement for avian acute toxicity testing via the inhalation route. As a consequence, exposure estimates based on external inhaled dose cannot be compared directly to effects data from the same route. Typically, available avian acute toxicity information is for single oral dose (gavage) and short-term dietary dose protocols. Therefore, to assess the potential risk of inhalation exposure, a method to relate inhalation exposure to an oral dose equivalent is needed.

An option submitted to the SAP in 2000 was to use the relationship between rat acute oral and acute inhalation LD_{50} values to establish a route equivalency factor. This factor would then be applied to avian inhalation dose estimates to estimate an oral dose equivalent exposure for subsequent comparison with avian oral dose acute toxicity endpoints. As summarized in the SAP report (2000), concerns were expressed that directly applying information from the rat data analysis to birds would not account for differences between the physiology of mammals and birds. Subsequently, the Agency evaluated the differences between avian and mammalian respiratory

physiology that might be considered in establishing a more taxonomically appropriate route equivalency factor. Appendix D includes a comparison of basic aspects avian and mammalian lung physiology and how these differences may influence the bioavailability of inhaled pesticide through taxonomic differences in diffusion rate across the pulmonary membrane. The Appendix presents a table of pulmonary membrane diffusion rate estimates for birds and mammals that indicates that the relative diffusion rates across the pulmonary membrane (Q_a/Q_m) would be between 2.4 and 3.4 times greater in birds than in mammals of similar body weights (weight range 1 to 2,000 g). These differences in diffusion rate can be used to modify the relationship of oral to inhalation toxicity endpoints in mammals to produce a route equivalency factor F_{re} that would at least account for the expected higher diffusion rates across avian pulmonary membranes.

$$F_{re} = \frac{oral\,LD_{50(mammal)}\,mg/kg\left(Q_a/Q_m\right)}{inhalation LD_{50(mammmal)}\,mg/kg} \qquad (3\text{-}52)$$

where,

F_{re} = the avian route equivalency factor

Q_a/Q_m = the ratio of avian to mammalian pulmonary membrane diffusion rates from Appendix D.

The route equivalency factor is then applied to estimated avian inhalation exposures to derive an estimate of the equivalent oral dose as follows:

estimated avian equivalent oral dose mg/kg = (estimated inhalation dose mg/kg)(F_{re}) (3-53)

Remaining uncertainties with this approach includes the extent to which physiological and biochemical aspects of the avian and mammalian lung not taken into consideration could over or under-estimate the equivalency factors. For example, there are likely differences in vascularization of mammalian and avian lung that may influence overall diffusion rates of xenobiotics and there is the potential for differences in enzymatic activity in lung tissue that may affect chemical rates of chemical transformation. These issues serve for a potential of future research and model development because these uncertainties could significantly impact overall exposure and risk estimates.

7. Next Steps for Inhalation Exposure Model

a. Examination and Comparison of Alternative Air Concentration Models with Available Air Measurement Data

Initial limitations of the air model include the assumption that equilibrium conditions exist. Consequently the rate of change in exposure as a function of changing meteorological conditions on air concentrations can not be determined. The model also cannot be applied to situations

where pesticides are applied to soils with little or no ground cover; an important limitation because many volatile pesticides such as soil fumigants, are applied to non-vegetated soils. Finally, the model is limited in the ability to address exposures at varying heights within the canopy.

Appendices E and F present efforts to over come some of these limitations, examining models for estimating air concentrations in the canopy and estimating air concentrations above bare-ground following pesticide application. This effort will focus on the determination of the relative predictive performance of each of the models under a variety of pesticide types, application scenarios, crop canopy types, and meteorological conditions, as available data allow.

b. Sensitivity Analysis

Sensitivity analyses of the models will be undertaken to determine the relative contributions of input variables to model uncertainty and results variation. These analyses will inform guidance for preparing risk characterization and provide insights for prioritizing future research.

G. Model for Dermal Exposure

Existing assessment methods for pesticide risks to avian wildlife do not consider the potential for exposure via dermal contact. The work of Driver et al. (1991) suggests that dermal contact with pesticides may, in some circumstances, contribute significantly to acute pesticide risks to birds. Furthermore, lines of evidence from fundamental principles of toxicokinetics and surface to volume ratios suggest that the dermal route can contribute significantly to total dose in terrestrial animals. Existing assessment methods do not include a quantitative evaluation of the potential for pesticide exposure via dermal contact and risk assessments assume that avian wildlife risks from dermal exposure to pesticides are inconsequential.

There are a number of challenging opportunities to consider in the dermal route in avian risk assessments. These include 1) development of an assessment method that can be based on existing environmental fate and effects testing, and 2) relating pesticide exposure via the dermal route to toxicity data generated through oral exposure testing methods. These challenges can be effectively met through the consideration and incorporation of existing Agency methods for accounting for dermal exposure, effects, and risk from other programs.

1. General Dermal Exposure Model

The general dermal exposure model considers two pathways: 1) direct interception of applied material during pesticide application and 2) incidental contact with dislodgeable pesticide residues on treated foliage. The general model does not address dermal exposure through contact with soil, nor with surface water, routes that can be incorporated in subsequent model versions.

For both routes modeled, the exposure is expressed on external dose (mass on animal surface) rather than an absorbed dose. The mathematical representations of the models are as follows:

Dermal Interception of Applied Material

$$IDD = \frac{A_{rate} SA_{intercept}}{BW} \tag{3-54}$$

where:

IDD = Intercepted Dermal Dose mg/kg
A_{rate} = application rate from label converted to mg/m^2
$SA_{intercept}$ = exposed surface area of bird intercepting applied pesticide (m^2) (See section on SA for further information)
BW = bird body weight (kg)

Incidental Dermal Contact with Dislodgeable Foliar Reside

$$IDCD = \frac{C_{plant} F_{dfr} R_{foliar\,contact} SA_{foliar\,contact} TC}{BW} \tag{3-55}$$

where:

IDCD = Incidental Dermal Contact Dose mg/kg
C_{plant} = concentration of the pesticide in crop foliage at time t (mg/kg) **(See section -C_{plant} --for further information)**
F_{dfr} = Dislodgeable foliar residue adjustment factor (kg/m^2) (See section on F_{dfr} for further information)
$R_{foliar\ contact}$ = rate of foliar contact (m^2 foliage/hr/m^2 body surface) (See section on $R_{foliar\ contact}$ for further information)
$SA_{foliar\ contact}$ = surface area of bird in contact with foliage (m^2) (See section on SA for further information)
TC = residue transfer coefficient
BW = bird weight (kg)

Surface Area of Birds for Interception ($SA_{intercept}$) and Foliar Contact ($SA_{foliar\ contact}$)

The total surface area of a bird is calculated using the allometric equation for relating bird body weight to surface area (USEPA, 1993):

$$SA_{total} = \frac{\left(BW(1000)\right)^{0.667}}{1000} \tag{3-56}$$

where,

BW = bird weight in kg

The dermal interception model assumes that pesticide deposition occurs in a manner consistent with a horizontal surface in the treatment area. Therefore, surface area calculation of a bird for the interception model assumes that the upper half of the bird in the field is exposed:

$$SA_{intercept} = SA_{total}\,0.5 \tag{3-57}$$

where: SA_{total} is the total bird surface area (m^2)

The dermal incidental contact model predicts transfer of pesticide residues from foliage to the bird foot and lower leg. The model does not include transfer of residues to wing patch or overall bird surface The surface area calculation for dermal exposure of birds for the interception model uses a point estimate of leg/foot surface area of 7 percent of the total body surface (USEPA, 1993):

$$SA_{foliar\,contact}\,(m^2) = SA_{total}\,0.07 \tag{3-58}$$

C_{plant} Concentration of Pesticide on Treated Foliage

This residue is linked to the randomly selected time zero residues used for broadleaf foliage in the assessment of dietary exposure and the dissipation calculations for that route of exposure to serve as the basis for pesticide concentration at time step T in the exposure period.

F_{dfr} Dislodgeable Foliar Residue Adjustment Factor

Dislodgeable foliar residues are assumed to be a fraction of the total residues in a plant. In addition, total residues are commonly expressed in terms of mass of pesticide per unit fresh mass of vegetation, while dislodgeable residues are commonly expressed in terms of mass of pesticide per unit surface area of the vegetation. A factor to relate total residues (distributed at time zero and dissipated over the course of the model run) to corresponding dislodgeable residues is established by comparing measured total and dislodgeable residues immediately following pesticide application:

$$F_{dfr} = \frac{DPR}{TPR} \tag{3-59}$$

where,

DPR = Dislodgeable pesticide residues (mg/m^2) and are from measured data immediately following pesticide application to the target crop and reported in

submissions to the Agency.

TPR = Total pesticide residues (mg/kg) and are from measured data immediately following pesticide application to the target crop reported in submissions to the Agency.

$R_{foliar\ contact}$ Foliar Contact Rate

The foliar contact rate is the surface area of vegetation that is contacted by a given surface area of a bird over the course of a time step. Experimental measurements of such contact rates for birds have not been identified in the literature to date. In the absence of such data specific for birds, the use of foliar contact data for other organisms has been explored. For its field worker risk assessment, data from field dosimetry studies are used to establish foliar contact rates for different parts of field workers' bodies. Appendix G presents a table of values used in evaluating dermal exposure to workers *via* incidental foliar contact. These contact values are estimates based on data collected in field trials for measurements of dislodgeable foliar residues and recovery of residues from field-worker body parts. Once residues are known on vegetation as mass per unit area, and recovered residues are known for mass of pesticide present on specific body parts of workers, the rate of foliar contact for the body part necessary to achieve the observed mass of residues on that body part at the end of the exposure period can be estimated.

In the absence of data specific to incidental foliar contact for birds, the model presently makes use of the data in Appendix G to develop a surrogate foliar contact rate. As mentioned previously, the model quantifies incidental contact exposure to the foot/lower leg as it is assumed that incidental contact might be the most significant for birds as they move about the foliage while foraging. Consequently, a surrogate value from the data in Appendix G (picker hands) was selected to represent a contact rate functionally equivalent to a bird foot grasping vegetation. The range of mean contact values for the picker hand wash measurements, as they relate to foliar contact reported in Appendix G, is 11.9 to 5,050 cm^2/hr. The model currently employs the value of 5,050 cm^2/hr. This value is not adjusted for duration of contact, as the avian exposure model is based on an hourly time step.

Naturally, the total foliar contact rate for pickers' hands cannot be used without adjustment for the relative surface area differences between pickers and birds. Thus, the contact rate measurement selected from Appendix G (5,050 cm^2/hr) is normalized for hand surface area. A typical surface area value for adult male hands (USEPA, 1997) of 0.084 m^2 (840 cm^2) was used to make this normalization:

$$R_{foliar\ contact} = \frac{5050 cm^2{}_{foliage}/hr}{840 cm^2{}_{body\ surface}}$$

$$= 6.01 cm^2{}_{foliage}/hr/cm^2{}_{body\ surface}$$

$$= 6.01 m^2_{foliage} / hr / m^2_{body\ surface} \quad (3\text{-}60)$$

Upon initial inspection, the surrogate approach contact rate for birds appears to yield a small estimate of foliar contact, given a bird's hourly activity during foraging. This is a product of the methodology incorporated in the dosimetry studies upon which the calculations are based. As stated earlier, measured foliar residues and measured body part residues are used to estimate a contact rate. There is a practical limit to the method for estimating the total foliar area contacted. A principal issue is the potential for the saturation of the receiving body surfaces with pesticide residue. Once saturated, the ability for a body surface area to retain additional contacted dislodgeable residue is reduced. The point of saturation of the body surface would constitute an upper bound of residue measurements on that body surface. Because foliar contact rates are calculated by comparison of measured dislodgeable residues on foliage with measured residues on the body surface and the measurement of body surface residues is limited to an upper bound of saturation, the method may underestimate the true foliage contact rate over time. The principle of saturation of body surface is applicable to birds and has the same potential effect of underestimating true foliage contact rates. However, using the saturation point as an upper limit of measured pesticide on the body surface to estimate an "effective" foliage contact rate avoids situations where organisms in the field are estimated to be accumulating pesticide residues at unreasonable rates (e.g., small birds, contacting a high amount of foliage; accumulating residues far in excess of the body surface saturation limit and perhaps in excess of body weight).

Additional study would clearly improve the approach for establishing a contact rate. Human dosimetry is not likely optimal for estimating bird contact. The assumption of transfer of residues from foliage to bird body surfaces equivalent to the transfer to human body surfaces represented in available field studies warrants investigation. Similarly, the assumption of equivalent retention of dislodged residues between bird and human body surfaces should be empirically determined. Finally, assumption that only lower leg and foot exposure are appropriate to model, not addressing other avian body surfaces as additional routes, should be investigated.

2. Transfer Coefficient (TC)

The model allows for a transfer coefficient to describe the portion of dislodgeable residues associated with a contacted area of foliage that can be transferred to the body surface. It should be noted that existing $R_{foliar\ contact}$ values are based on the complete transfer of residues. The model currently assumes complete transfer of residues from the estimated foliar area contacted and so sets the TC value at 1.0. However, it is anticipated that as foliar contact data are developed over time, the TC value can be made avian specific and more accurately reflect the transfer of residues from plant to animal.

3. Parameterization

Table 3-6. Dermal model parameters

Parameter	Units	Description	Recommended Value
A_{rate}	mg/m^2	labeled rate of pesticide a.i. application	User defined
SA_{total}	m^2	total bird surface area	$SA_{total} = \frac{(body\ weight*1{,}000)^{0.667}}{1{,}000}$
$SA_{intercept}$	m^2	exposed surface area of bird intercepting applied pesticide	$SA_{intercept} = 0.5\ (SA_{total})$
$SA_{foliar\ contact}$	m^2	surface area of bird for foliar contact (assumed to be foot and lower leg)	$SA_{foliar\ contact} = (SA_{total})\ (0.07)$
body weight	kg	bird body weight	see text on generic bird types
C_{plant}	mg/kg	pesticide concentration in foliage	based on dietary residue distributions
F_{dfr}	kg/m^2	dislodgeable foliar residue adjustment factor	$F_{dfr} = \frac{\text{Dislodgeable pesticide residues mg/m}^2}{\text{Total pesticide residue mg/kg}}$
Dislodgeable pesticide residues	mg/m^2	measured dislodgeable pesticide residues for crop sampled as close as possible to day of application	user defined from available HED studies
Total pesticide residue	mg/kg	total pesticide residue on crop on day of application	user defined from available data corresponding to dislodgeable studies or from dietary residue distributions
$R_{foliar\ contact}$	m^2 foliage/hr/m^2 body surface	rate of organism foliar contact	current default from field worker data for hands (6.01)
TC	unitless	residue transfer coefficient	current default is 1.0

4. Scenarios for Consideration of Pesticide Exposure Through Dermal Exposure

Dermal exposure from applied pesticide droplet is considered for the first exposure time

step immediately following the pesticide application and for both aerially and ground applied sprays. It is assumed that a suspended droplet will have either settled or cleared from the application area by the next time step, 60 minutes after application. For aerially applied spray, all individual birds predicted to be in the field at the time of application are subject to dermal exposure from applied pesticide droplet. This assumption is based on an expected rapid rate of application by aerial equipment, with little opportunity for individuals to leave the field during application. However, for ground applied sprays, dermal exposure to pesticide droplet is limited to those individual that are predicted by the model to be on the field at the time of application and for situations where ground spray is not made to bare ground. The limitation to in-field residents is based on an expectation that non-territory holding individuals will have the opportunity to exit the field in advance of the application equipment, but field residents will remain on field. The limitation to non-bare ground applications is predicated on an assumption that even residents will flush before application equipment because no vegetative cover is present.

Dermal contact with foliage is modeled for every bird and time step where the model predicts the individual to be present in the treated field feeding. During non-feeding periods for both edge and resident species, dermal exposure is assumed zero. Edge species are assumed to be off the field, and resident species, activity is assumed to be minimal, resulting in relative low contact with vegetation.

5. Relating External Dermal Dose to Oral Dose Equivalents

Currently, the Agency does not have a data requirement for avian acute toxicity testing via the dermal route. As a consequence, exposure estimates based on external dermal dose cannot be compared directly to effects data from the same route for most pesticides. Typically, only available avian acute toxicity information is for single oral dose (gavage) and short-term dietary dose protocols. Therefore, to assess the potential risk of inhalation exposure, a method to relate dermal exposure to an oral dose equivalent is needed in situations where the available data do not include a dermal toxicity test.

In situations where avian dermal and oral LD_{50} data are available for a bird species, a route equivalence factor (F_{red}) is calculated as follows:

$$F_{red} = \frac{LD_{50(avian\,oral\,for\,species\,x)}}{LD_{50(avian\,dermal\,for\,species\,x)}} \qquad (3\text{-}61)$$

In most cases, both oral and dermal LD_{50} data are not available for a given pesticide. Consequently, the potential for developing an empirical model to establish a relationship between avian acute oral and avian acute dermal toxicity measurements that could be used when paired effects data are not available was investigated. Data are available for a subset of pesticides that allow comparisons of acute oral and dermal LD_{50} measurements (Appendix H). In addition to a correlation of dermal LD_{50} with oral LD_{50}, other physical chemical properties were considered, in

a manner consistent with methods reported in Mineau (2002), to investigate if these variables could provide for a more robust relationship between oral and dermal observations. Appendix H provides the results of these analyses. Based on this work, the following equation was adopted for the revised model to estimate a dermal LD_{50}, when only oral LD_{50} data are available:

$$\log LD_{50(dermal)} = 0.84 + 0.62\left(\log LD_{50(oral)}\right) \quad (3\text{-}62)$$

This relationship is than used in the model to estimate a dermal route equivalency factor (F_{red}) as follows:

$$F_{red} = \frac{LD_{50(avian\ oral)}}{10^{\left(0.84+0.62(\log LD_{50(oral)})\right)}} \quad (3\text{-}63)$$

The route equivalency factor is then applied to estimated avian dermal exposures to derive an estimate of the equivalent oral dose as follows:

estimated avian equivalent oral dose mg/kg = (estimated dermal dose mg/kg)(F_{red}) (3-64)

There is likely considerable uncertainty in this approach because of the poor correlation established between available measurements of acute oral and acute dermal toxicity. The correlations were not improved when other physical/chemical properties were considered. However, the simple correlation models used to test for physical/chemical property influences were not mechanistic. It is possible that more predictive models may be developed in the future that relate pesticide physical/chemical properties to rates of absorption across, and metabolism within, avian skin tissue. A more complete understanding of such mechanisms affecting bioavailability may aid in the establishment of more robust predictive models of avian dermal toxicity. These issues remain topics for further research and future model development.

6. Sensitivity Analysis

Sensitivity analyses are planed to determine the relative contributions of model variables to risk estimates. It is anticipated that this analyses will provide guidance for preparing risk characterization descriptions and provide insight for the agency and other interested parties to optimize efforts for any future research.