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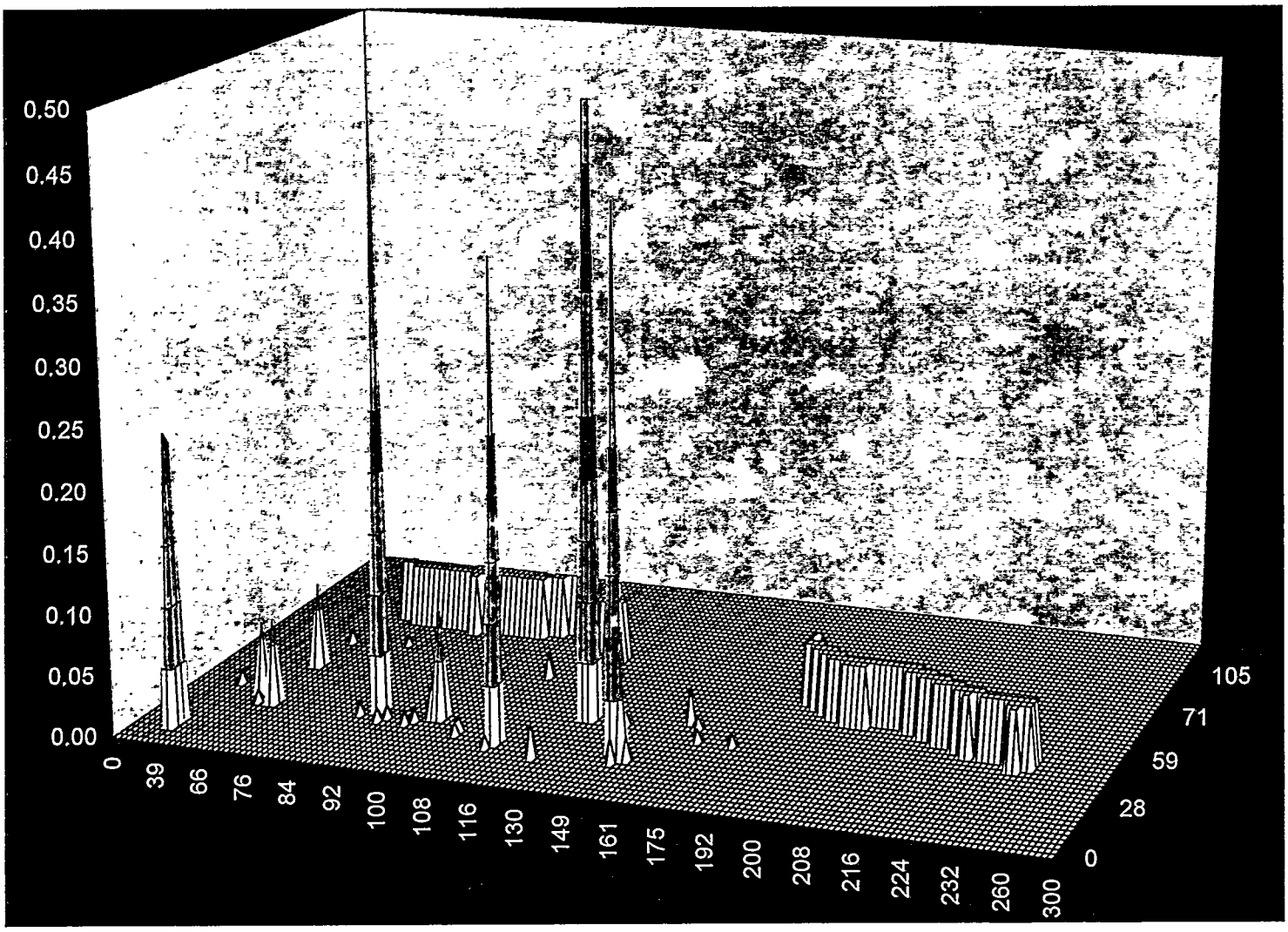
Documentation of the Ecological Risk Assessment Computer Model ECORSK.5



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Edited by Hector Hinojosa, Group CIC-1
Prepared by Carolyn Hedrick, Group ESH-20

Cover: The cover figure depicts "partial hazard quotients" (multicolored prisms), which is one measure of "ecological risk," for one of many contaminants assessed for potential impact to the American peregrine falcon. The figure illustrates how the integration of ECORSK.5 with a geographic information system enables users to present risk indices on a spatial basis. The two yellow blocks are depictions of nesting habitats to which the hazard quotients contribute.

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Documentation of the Ecological Risk Assessment Computer Model ECORSK.5

*Anthony F. Gallegos**
*Gilbert J. Gonzales***

**Earth and Environmental Science Group (EES-15).*
***Ecology Group (ESH-20).*

Los Alamos
NATIONAL LABORATORY
Los Alamos, New Mexico 87545

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Documentation of the Ecological Risk Assessment Computer Model ECORSK.5

Anthony F. Gallegos and Gilbert J. Gonzales

ABSTRACT

The FORTRAN77 ecological risk computer model—ECORSK.5—has been used to estimate the potential toxicity of surficial deposits of radioactive and non-radioactive contaminants to several threatened and endangered (T&E) species at the Los Alamos National Laboratory (LANL). These analyses to date include preliminary toxicity estimates for the Mexican spotted owl, the American peregrine falcon, the bald eagle, and the southwestern willow flycatcher.

This work has been performed as required for the Record of Decision for the construction of the Dual Axis Radiographic Hydrodynamic Test (DARHT) Facility at LANL as part of the Environmental Impact Statement. The model is dependent on the use of the geographic information system and associated software—ARC/INFO—and has been used in conjunction with LANL's Facility for Information Management and Display (FIMAD) contaminant database. The integration of FIMAD data and ARC/INFO using ECORSK.5 allows the generation of spatial information from a gridded area of potential exposure called an Ecological Exposure Unit. ECORSK.5 was used to simulate exposures using a modified Environmental Protection Agency Quotient Method. The model can handle a large number of contaminants within the home range of T&E species. This integration results in the production of hazard indices which, when compared to risk evaluation criteria, estimate the potential for impact from consumption of contaminants in food and ingestion of soil. The assessment is considered a Tier-2 type of analysis.

This report summarizes and documents the ECORSK.5 code, the mathematical models used in the development of ECORSK.5, and the input and other requirements for its operation. Other auxiliary FORTRAN 77 codes used for processing and graphing output from ECORSK.5 are also discussed. The reader may refer to reports cited in the introduction to obtain greater detail on past applications of ECORSK.5 and assumptions used in deriving model parameters. A FORTRAN 90 version of the code is under development.

Introduction

In 1996 the custom FORTRAN code ECORSK was developed to estimate the potential for impact from contaminants to threatened and endangered (T&E) species at the Los Alamos National Laboratory (LANL). To date four T&E species—the Mexican spotted owl, the American peregrine falcon, the bald eagle, and the southwestern willow flycatcher—have been assessed. Results of these assessments can be found in the following reports: Gonzales et al. (1998a, b, and c), Gonzales et al. (1997), and Gallegos et al. (1997a and b). The code integrates a contaminant database maintained by LANL's Facility for Information Management and Display (FIMAD) with a geographical information system (GIS) and computes spatially-dynamic hazard indices (HIs) over broad geographical areas using a modified Environmental Protection Agency Quotient Method (EPAQM). Figure 1 is a conceptual model of the integration of ECORSK.5, FIMAD, and the GIS as well as other routines that are discussed later. The current version of the code, ECORSK.5, accommodates multi-site and/or multi-contaminant ecological risk assessments and can be modified for other sites where a large number of different contaminants of concern (COCs) are distributed over a large area. The modes of entry or pathways of contaminants modeled in ECORSK.5 are food consumption and soil ingestion, and the code can be modified to include additional pathways.

The FIMAD contaminant database includes two-dimensional Universal Transverse Mercator (UTM) space coordinates for many contaminant concentrations and locations within the LANL reservation using the GIS software ARC/INFO. ECORSK.5 output can be superimposed onto specific wildlife habitats such that risk indices are spatially dynamic.

Mapping the spatial components was accomplished by gridding nesting habitats and foraging areas (or home ranges), which together comprise Ecological Exposure Units (EEUs), and by developing methods by which ECORSK.5 randomly assigns nest sites and differentiates the spatial components. Nest site selection by ECORSK.5 is random using Monte Carlo methods, or alternatively, nests can be specifically assigned to particular grid cells. For example, nest sites might be assigned to contaminated grid cells to compare with random nest assignments to test for the effect of aggregate contaminant locations. The occupancy term, and therefore simulated foraging time, of a T&E species on grid cells may be set to equal on all grid cells, or expected occupancies based on greater or lesser use of an area can be modified using enhancement factors included as part of the input to the model. The model currently simulates foraging on both contaminated and non-contaminated grid cells to add more realism to an ecological risk assessment. Great utility is made of GIS input to ECORSK.5, which must be integrated with other input parameters for proper execution.

Finally, the home range (HR) geometry for a given nest site can be varied both for shape and alignment with important geographical features within the EEU. Other features of ECORSK.5, including important analytical and diagnostic output, will be discussed in the following sections of this report.

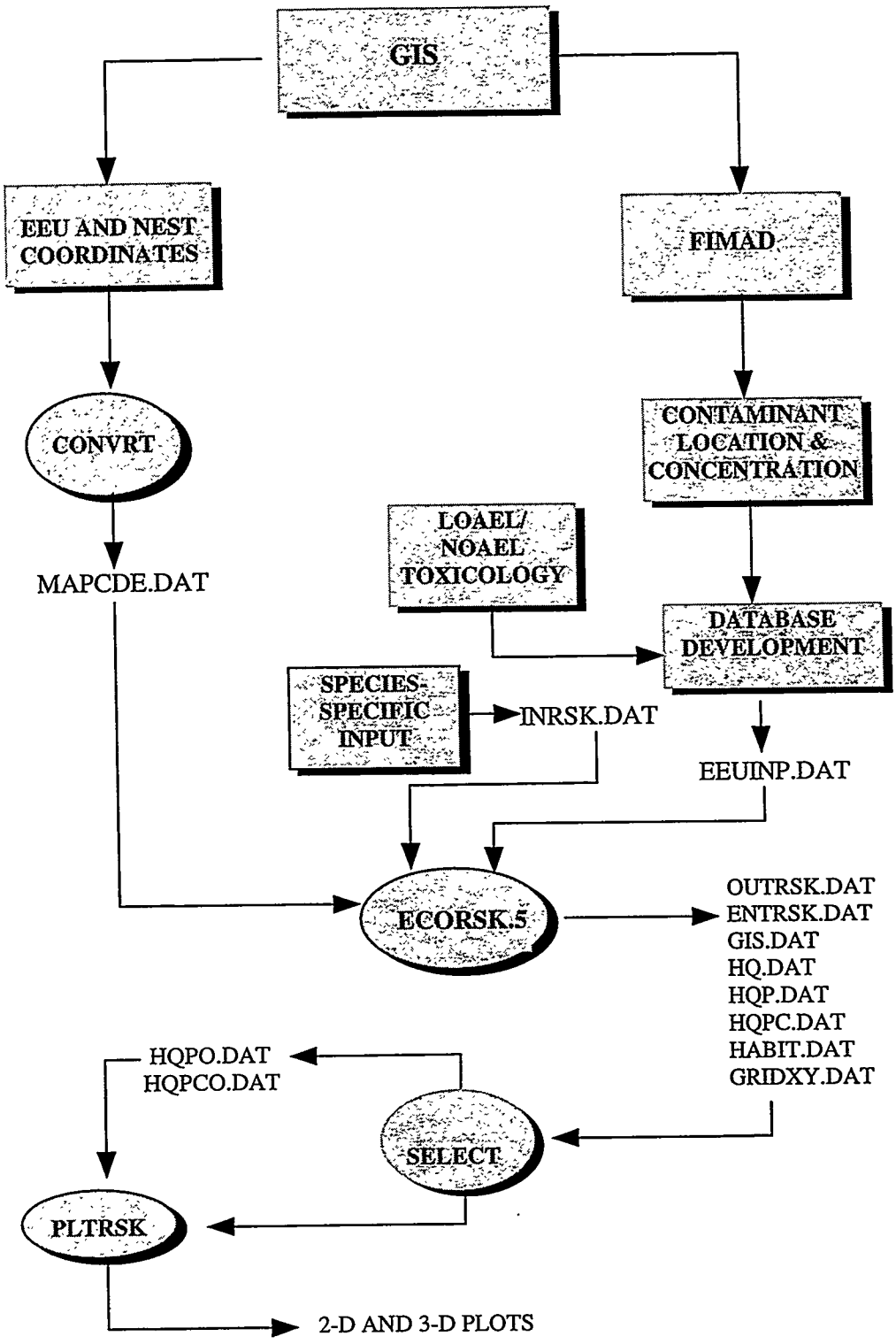

Figure 1. **Schematic of strategy for integrating FORTRAN code with GIS and FIMAD data.**

1.0 Development of the EPAQM Algorithm

1.1 Basic EPAQM

The EPAQM in its simplest form involves the ratio of an organism's consumptive exposure dose (mg COC/kg-body weight/day) to the toxicity reference value (TRV) for a given contaminant with the same units:

$$HQ = E/(TRV), \quad (1)$$

where

HQ = hazard quotient,

E = exposure dose (mg/kg-body weight/day), and

TRV = toxicity reference value (mg/kg-body weight/day) [INPUT].

HQ values exceeding unity may be considered potentially unacceptable risk and may indicate the need to more fully assess the exposure by more refined means. Both E and TRV refer to an ingested dose from food, water, soil, and other media, although only the two dominant pathways—food consumption and soil ingestion—have been utilized thus far.

1.1.1 Food Intake

The exposure E can be generally estimated from a food consumption rate (I_f, kg/day) and, if known, the concentration of COC in the food (C_{fd}, mg/kgdwt-food), so that Eq. (1) may be rewritten as

$$HQ = I_f C_{fd}/(BW \times TRV), \quad (2)$$

where

I_f = food consumption, kgdwt/day,

C_{fd} = contaminant concentration in food, mg/kgdwt, and

BW = body weight of organism, kgfwt.

1.1.2 Soil Ingestion

If the COC is in another media such as soil, then the fraction of diet which is soil (F_s) can be used to form the relationship:

$$HQ = F_s I_f C_s/(BW \times TRV), \quad (3)$$

where

F_s = fraction of food intake as soil [INPUT], and

C_s = COC concentration in surficial soil, mg/kgdwt [INPUT].

Currently, ECORSK.5 is set to estimate HQs from contaminated soils or sediments as a major source of COC intake in the LANL terrestrial environment.

1.2 Multi-Site EPAQM Involving Soil or Sediment Ingestion

Equations 1, 2, and 3 assume a single feeding location and a single concentration of one COC. However, if ingestion occurs over multiple feeding sites that do not have equal COC concentrations, then a summation of HQs over all feeding sites is needed. An occupancy factor (O) must be used for each feeding site, which estimates the ratio of the feeding interval at a given site to the total feeding time over all sites. Assuming that only one COC is present, the cumulative HQ over all sites, which is called a partial hazard index (pHI) may be estimated by modifying Eq. (3) as follows:

$$pHI = F_s I_f/(BW\ TRV) \sum_{i=1}^{ncs} Cs_i O_i\ ENH_i, \quad (4)$$

where

pHI = partial hazard index (cumulative HQ over all grid cells for <u>one</u> contaminant),

Cs_i = concentration of COC on the soil surface for the *ith* feeding site, mg/kgdwt

[INPUT],

O_i = occupancy factor for the *ith* feeding site,

ENH_i = enhancement factor for the *ith* feeding site [INPUT], and

ncs = total number of nest sites (nest sites) [PARAMETER].

Equation 4 shows that HQs estimated for each feeding site, when summed, become a pHI for the organism of concern. The term "partial" in this case refers to the fact that only one COC is still involved. (Note: "Partial" can also refer to the sum of HQs for all COCs at one site.) If the COC concentration is the same at each site, then Eq. (4) reduces to Eq. (3) because the sum of the occupancy factors must equal unity. The occupancy factors estimate the fraction of the food intake from each site and should account for any obstructions such as paved surfaces, fences, roads, etc., which make sites more or less suitable for feeding activities than others. The latter is accomplished through the use of enhancement factors (ENH) that either increase or decrease feeding times. ENH can also be used to account for any non-linear response between feeding time and the amount of food consumed on a site-by-site basis.

1.3 Multi-Site, Multi-COC EPAQM Involving Soil or Sediment Ingestion

If more than one COC is present in a multi-site feeding scenario, then Eq. (4) can be modified to account for this condition:

$$HI = (F_s I_f / BW) \sum_{i=1}^{ncs} O_i \, ENH_i \sum_{j=1}^{ncoc} Cs_{i,j} / TRV_j, \quad (5)$$

where

$Cs_{i,j}$ = COC concentration of soil/sediment, mg/kgdwt, for the *ith* feeding site,

and the *jth* contaminant,

TRV_j = toxicological reference value, mg/kg-body weight/day, for the *jth* COC, and

ncoc = total number of different COCs found over all nesting sites.

Equation 5 contains not only pHI information with respect to feeding site, but also partials of specific COCs within and among all sites. When the pHI for all COCs and the pHI for all sites are summed into a single HI, then it no longer is "partial," but represents the ultimate (most conservative) HI. Since not all sites contain the same number of COCs nor the same COCs, the index value (ncoc) represents the number of different COCs found over all sites. Hence, sites without a specific COC must be set to zero within the summation. Equation 5 is the basic algorithm that has been used in ECORSK.5 to estimate HI for T&E species.

1.4 Food Consumption Contaminant Pathway

Although soil ingestion is believed to be the dominant pathway for exposure of T&E species to contaminants, food consumption can play a relatively large role depending on the circumstances. This is true especially for COCs that are subject to bioaccumulation or biomagnification of contaminants. Bioaccumulation is defined as the transfer of a contaminant from soil to organism over time and the deposition and retardation of the contaminant in the organism based on an affinity of the contaminant for an organ or tissue of a particular type. Biomagnification is defined as the process by which contaminants are transported to a receptor organism via its food chain and the coincidental increase in contaminant concentration at one or more trophic levels. For COCs expected to exhibit either bioaccumulation or biomagnification within a given animal,

Equation 5 may be modified to accommodate these effects as

$$HI = I_f/BW \sum_{i=1}^{ncs} O_t ENH_i \sum_{j=1}^{ncoc} [F_s + (1-F_s)\, BMF_i]\, Cs_{i,f}/TRV_i \quad (6a)$$

or

$$HI = I_f/BW \sum_{i=1}^{ncs} O_t ENH_i \sum_{j=1}^{ncoc} [F_s + (1-F_s)\, BAF_i]\, Cs_{i,f}/TRV_i \quad (6b)$$

where

BAF_i = bioaccumulation factor via soil or sediment intake for the *jth* contaminant and

BMF_i = biomagnification factor via food chain transport for the *jth* contaminant.

The specific formulation of BMFs or BAFs associated with prey consumption as stated above are inferred through the following differential equation between COC uptake and prey body burden of COC and other relationships given below:

$$DQ/DT = I_c - \lambda Q , \quad (7a)$$

where

Q = body burden of a COC in prey organism, mg,

I_c = intake rate of COC into the body, mg/day, and

λ = excretion rate, day $^{-1}$, of COC back into the environment including fecal and other routes i.e., urinary, exhalation, etc.

At equilibrium: $I_c = \lambda Q$ (7b)

and division of both sides by the body weight yields: $I_c/BW_p = \lambda C_{ff}$, (7c)

where

BW_p = body weight of prey, kgfwt,

C_{ff} = COC concentration in prey, mg/kgfwt,

and

$$C_{ff} = I_c/(\lambda\, BW_p). \quad (7d)$$

But the contaminant intake (I) for the prey organism is

$$I_c = I_{fp} F_s C_s, \text{ so that } C_{ff} = I_f F_s C_s/(\lambda\, BW_p), \quad (7e)$$

where

I_{fp} = food intake by prey, kgdwt/day

but

$$I_{fp} = C_p\, BW_p^{\,y}. \quad (7f)$$

As described in another report (Gallegos et al.,1997a) for mammal, reptile, and bird species

$$C_{ff} = C_s\, [C_p\, BW_p^{\,y-1}\, F_s/\lambda] , \quad (7g)$$

where

C_p = intake proportionality constant, gdwt, for prey, and

y = constant exponent for prey.

If both sides of Eq. 7g are divided by the dry weight fraction of the animal in question, it yields the dry weight concentration of contaminant in the prey:

$$C_{fd} = C_s[C_p\, BW_p^{\,y-1}\, F_s/(\lambda\, dwf)] , \quad (7h)$$

where

C_{fd} = COC concentration in the prey, mg/kgdwt, and

dwf = dry weight fraction of the prey.

The terms within the brackets of Eqs. 7g and 7h may be considered estimates of the BAFs and BMFs used in Eqs. 6a and 6b:

$$BAF, BMF \cong [C_p\, BW_p^{\,y-1}\, F_s/(\lambda\, dwf)]\, [INPUT] \quad (7i)$$

$$BAF, BMF \cong [C_p\, BW_p^{\,y-1}\, F_s/\lambda\,], [INPUT] , \quad (7j)$$

which are applicable for dry weight and fresh weight comparisons of prey tissue COC concentrations to soil COC concentrations, respectively. In cases where the predator does not consume and/or digest all of the prey tissue, adjustment for actual consumption can also be included in the formulation. Finally, the additional COC intake resulting from soil ingestion apart from prey consumption is also included in Eqs. 6a and 6b, but can be excluded from consideration by input specifications into ECORSK.5 if necessary. These estimates are shown to be directly proportional to body weight and inversely related to the

biological excretion rate from the body and the dry weight fraction when applicable. This can be represented as

$$\lambda = 0.693/TB_{1/2}\,, \qquad (7k)$$

where

$TB_{1/2}$ = the biological half-time of the COC in the prey.

Excretion rate data of this type are generally available for many COCs including radionuclides in a large number of species, or may be obtained from pharmacokinetic data via partition coefficients (Mordenti 1986). Both BAFs and BMFs must be related back to a COC concentration in soil for them to be compatible with the ECORSK.5 model which operates exclusively with soil COC concentrations (C_s) as shown in Eqs. 6a and 6b.

1.5 EPAQM for Radionuclides

Animal toxicity data for radionuclides are largely unavailable (Gonzales et al., 1998a), however it is important to use some means for comparing actual COC concentrations in the environment to benchmarks, i.e., COC concentrations, that are assumed to be indicative of potential harm to animals. In ECORSK.5, dose conversion factors recently developed by Amiro (1997) have been used to estimate nuclide-specific TRVs from the limit of 0.1 rad/day recommended by the International Atomic Energy Agency as protective of T&E species (IAEA 1992). The application of the EPAQM for radionuclide COCs involves a simplification of the EPAQM in Eq. 5 for multi-site and multi-COC conditions:

$$HI = \sum_{i=1}^{ncs} O_i\, ENH_i \sum_{j=1}^{ncoc} SC_{i,j}/(ESAL_j)\,, \qquad (8)$$

where

$SC_{i,j}$ = COC concentration in soil, pCi/kgdwt, for the *ith* nest site, and the *jth* radionuclide COC and

$ESAL_j$ = screening action level in soil, pCi/kgdwt, for the *jth* radionuclide COC.

Both radionuclide and non-radionuclide COCs are integrated in the ECORSK.5 to produce a cumulative HI, however, the model does have provision to separate contributions to the HI by site and by COC at any given site or over all sites (Gallegos et al., 1997a).

1.6 Estimation of Sediment Intake Fractions from Real Data for Use in the EPAQM

In some cases prey data may be available, and this allows for a more realistic estimate of potential impact to be made. Since ECORSK.5 has models for estimating exposure dose using concentrations of COCs in soil or sediment, the use of COC concentration in prey tissue simply entails expressing (back calculating) tissue concentrations as the fraction of diet made up of soil or sediment. For instance, Gonzales et al. (1998a) used the mean concentration of radionuclides in fish tissue, which is consumed by bald eagles, to compute the mean concentration in Rio Grande sediment. The sediment intake fraction in the daily food intake was expressed as:

$$F_{sed} = I_{sed}/I_{fp}\,, \qquad (8a)$$

where

F_{sed} = fraction of daily food intake comprised of sediment,

I_{sed} = sediment ingestion rate, kgdwt/day, and

I_{fp} = food consumption rate, kgdwt/day, based on gut content by prey,

where sediment ingestion rate (I_{sed}) is estimated as

$$I_{sed} = I_{pr}/C_{sed}\ , \qquad (8b)$$

where

I_{pr} = COC intake rate by predator, mg/day, and

C_{sed} = COC concentration in sediment, mg/kgdwt,

but

$$I_{pr} = I_{f\,p}C_t \qquad (8c)$$

and

C_t = COC concentration in prey viscera and muscle tissue, mg/kgdwt.

The bald eagle data were limited to radionuclide COCs in fish and river sediments (Fresquez et al., 1994), however the method is applicable to any COC if data is available. It should also be noted that any BAF or BMF effects are included in this formulation, so that these terms would be set to zero in Eqs. 6a and 6b.

1.7 Estimation of Other Parameters Used in the EPAQM Model

1.7.1 Daily Food Intake

The food intake term shown in Eqs. 6a and 6b is invariant for any animal used for an EPAQM determination. The body weight of a mature animal is used to estimate the daily food consumption rate (I_f) on a dry weight basis for mammal, bird, reptile, and amphibians (EPA 1993):

$$I_f = 0.0687\ BW^{0.886} \text{ for mammals,} \qquad (9a)$$

$$I_f = 0.0582\ BW^{0.651} \text{ for birds, and} \qquad (9b)$$

$$I_f = 0.0135\ BW^{0.773} \text{ for reptiles and amphibians.} \qquad (9c)$$

These relationships can be applied to general types of animals as shown, however, more specific relationships can be used if more precision is required.

1.7.2 Soil Intake Fraction

The amount of soil consumed concomitantly with food, expressed as a fraction (F_s) of food intake (I_f), that is used in Eqs. 6a and 6b and other relationships of the ECORSK.5 model is entered as an input parameter. A detailed discussion of the rationale and general estimation approach for this parameter is presented in a previous report (Gallegos et al., 1997a). For avian species, F_s may vary from less than 2% up to 30% depending on feeding habits. Similar variations also occur between mammalian and other species depending on their position within a given food web or food chain.

1.7.3 Occupancy Factor Estimation

1.7.3.1 Unweighted Occupancy Factors

Occupancy factors (O_i) for any grid area (i) of an EEU are estimated from input of these grid areas to the ECORSK.5 model. However, these factors are generally invariant for a given EPAQM assessment in the model because they are based on equal grid sizes throughout the EEU as supplied by ARC/INFO. Assuming equal grid size across a gridded HR of an animal, the following relationship is utilized for modifying occupancy estimates on a site-by-site basis as shown in Eqs. 6a and 6b and other relationships in the model:

$$O_i = A_i/\sum A_i\, ENH_I\ , \qquad (9d)$$

where

A_i = surface area, km^2, of the *ith* grid within the HR of a given animal.

The enhancement factor (ENH_i) is used to increase or decrease the use of any

ith grid within the HR of the animal in question.

1.7.3.2 Nest Site Weighted Occupancy Factors

Another weighting parameter can be superimposed on each grid area if the assumption is made that the relative probability of foraging is inversely related to the radial distance from its nest site or roosting area (Johnson 1996). Equation 9a may be modified as follows through the use of an exponential function:

$$O_i = A_i/\sum A_i \, ENH_i \; Exp\,(-R_i/R_c)\,, \quad (9e)$$

where

R_i = radial distance, m, of the *ith* grid from the grid center containing the nest site and

R_c = a scaling constant, m, for a given bird species [INPUT].

Scaling constants of 400 m, 350 m, and 2000 m were estimated from Johnson (1996) for the Mexican spotted owl, American peregrine falcon, and the bald eagle, respectively (Gallegos et al., 1997a, 1997b; Gonzales et al., 1998a). Scaling constants for non-avian species can be obtained in a similar manner.

2.0 Description of Input Instructions for Executing ECORSK.5 and Complementary Codes CONVRT, PLTRSK, and SELECT

ECORSK.5 estimates partial and total HQs and HIs, respectively, from GIS ARC/INFO-located contaminants for a given animal species from specified nest site locations. GIS mapping also locates the nest sites, and it is from these focal points that HQs and HIs are estimated using a number of requirements to be described below. The complimentary codes CONVRT, PLTRSK, and SELECT are utilized to transform, select, and provide graphics for the output files from ECORSK.5. Figure 1 shows how these codes are integrated. Figure 2 is an example of a PLTRSK-generated three-dimensional graphic.

2.1 File Requirements for ECORSK.5

The following files must be present to allow execution of ECORSK.5:

gis.dat [OUTPUT], unit = 4
outrsk.dat [OUTPUT], unit = 5
entrsk.dat [OUTPUT], unit = 6
inrsk.dat [INPUT], unit = 7
hqp.dat [OUTPUT], unit = 8
eeuinp.dat [INPUT], unit = 9
mapcde.dat [INPUT], unit = 10
hqpc.dat [OUTPUT], unit = 11
hq.dat [OUTPUT], unit = 12
habit.dat [OUTPUT], unit = 13
gridxy.dat [OUTPUT], unit = 14
river.dat [INPUT], unit = 15

The output files *hqp.dat*, *hqpc.dat*, *hq.dat*, *habit.dat*, and *gridxy.dat* have up to six lines of description on a column-by-column basis. ECORSK.5 requires that output files be created (at least with a dummy numerical value such as 1.0, etc.). All input files must be complete before execution of ECORSK.5 unless they are to be created by the user during execution (they also must be created as dummies if such is the case). The output file *gis.dat* is a verification copy of *eeuinp.dat* input data. The file *outrsk.dat* is a summary output file of input parameters and statistical output (HI, pHIs, etc.) from the run. The output file *entrsk.dat* is a copy of entered data from *inrsk.dat* and from *mapcde.dat*. A description of other output files will be presented in this section and subsequent sections as needed. If any files are missing

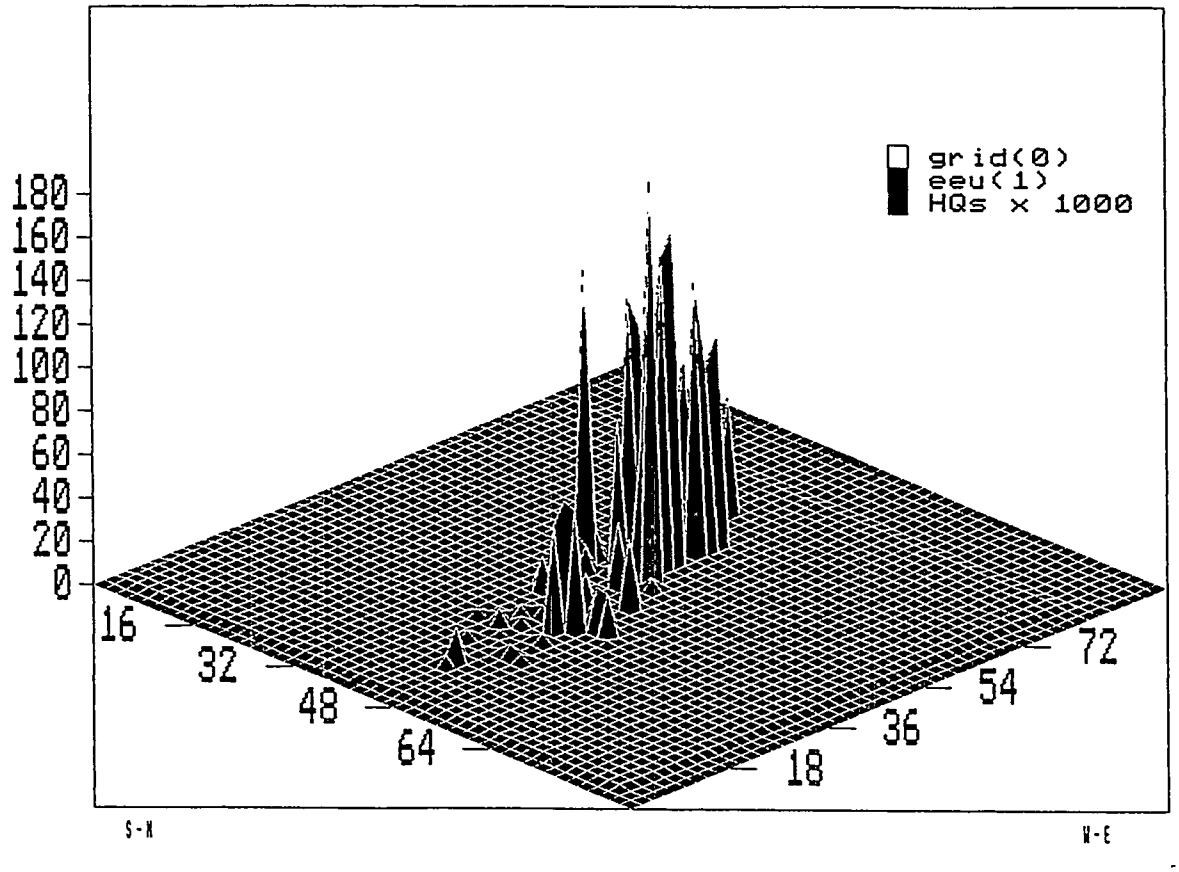

Figure 2. Example of PLTRSK-generated three-dimensional graphic.

during a run, a diagnostic error will give the unit number of the missing file(s).

2.2 Terminal Input Requirements for ECORSK.5

ECORSK.5 is executed using the command: RUN77 ECORSK.5. This command is followed by a series of input requests/options described in the following subsections. All input is free format unless specified differently.

2.2.1 Random Number Seed for Making Random Nest Selections on the Nesting Habitat

Entering random number request 'true' will default to a seed number of 1000, whereas 'false' results in a request for a user specified seed number, 'end' will terminate program. Note that single quotes ('') around the word are required.

2.2.2 Random Number Specification Option

A random number seed must be entered if 'false' was entered in Sec. 2.2.1. This causes the random number generator to start in a different sequence than when a seed of 1000 is used as a default. Any integer number may be entered, i.e., 234, 567, ... etc.

2.2.3 Run-time Information Specification

"Run-time" information such as the user name, date, or site description can be entered (50-character limit) to help identify each run specifically. Quotes are not required in entering this information.

2.2.4 Terminal Input Option (0, 1) for the Input Files *inrsk.dat, mapcde.dat,* and *eeuinp.dat*

Entering a value of "0" will signal that the user will be entering data from the terminal during execution and the data would be stored in the file *entrsk.dat* (if such is the case, a dummy file of *inrsk.dat* is required). Since output files such as *entrsk.dat,* which are located in the "dbos" directory, are overwritten each time that ECORSK.5 is executed, any output file that the user wants to save must be saved in a subdirectory outside of the "dbos" subdirectory. We suggest using a naming convention for subdirectories that is unique to the set of conditions, parameters, or scenario for which ECORSK.5 is executed. *Entrsk.dat* includes a copy of input data included in *mapcde.dat* for verification purposes (not used as part of *inrsk.dat* input file) which can be separated for use in future runs as *mapcde.dat.* If a value of "1" is entered, then complete files are assumed and the output file *entrsk.dat* serves as a copy of *inrsk.dat* and *mapcde.dat* for verification purposes only. Both *eeuinp.dat* and *mapcde.dat,* also needed for ECORSK.5 execution, will query the user for terminal input if complete files are not available. The user can use the query option to continue adding data to any input file during different sessions before execution, particularly when the amount of input required is too large for entering at one sitting. As a rule the latter two files are created before execution of ECORSK.5, and *entrsk.dat* is used for diagnostic purposes such as data verification and the detection of data input errors. Other output files, to be described later in this section, can also be used to locate input errors.

2.2.5 Echo Option (0, 1)

A value of "1" is entered if the user wants to see an on-screen listing of all file input parameters, otherwise a value of "0" should be entered. In general, this option is not used unless files are being created by the user at the terminal during execution and/or for debugging of input data errors because this option can be time consuming for the scroll to be completed.

2.2.6 COC Input Options (1, 2, 3)

Since both soil sample COC concentrations and soil background COC concentrations are required input, three options exist for HQ/HI determinations of all COCs present. Entering a value of "1" selects the use of the "Unadjusted Sample Mean" COC concentration. This results in the calculation of "Total Risk," which includes the contribution of both "background" COC values and elevated COC values. A value of "2" results in the calculation of "Background Risk" by using only background COC concentrations, whereas, an entered value of "3" results in

the calculation of "Adjusted Risk" by using background-corrected COC concentrations. In some cases, such as with organic COCs, background levels do not exist, while in other instances background values may not be available. A value of "1" is generally used when incomplete data and/or no background data is available. Background checks may also be used to estimate the contribution for some COC from waste disposal operations at a given site.

2.2.7 Nest Site Placement Strategy Options (1, 2, 3, 4, 5, 6)

A value of "1" will produce HI estimates of both contaminated and random nest sites. Hence, HI estimates will be estimated for grid cells within the nesting habitat that have COC(s) contamination as well as for nest sites that are randomly located within the nesting habitat that may or may not contain COCs. A value of "2" will produce HI estimates for COC-contaminated nest sites. A value of "3" will produce HI estimates for randomly-located nest sites. A value of "4" will produce HI estimates for specified nest site locations. A value of "5" will produce HI estimates for specified and randomly located nest sites, and a value of "6" will produce HI estimates for specified and COC-contaminated. Any combination of nest sites will lead to separate output for each case. Selected sites must be entered by the user as the last set of data in the *eeuinp.dat* input file to be described below. The last option is useful when HI estimates are desired for known nest locations, which may or may not contain COCs, or for other reasons.

2.2.8 Selected Nest Site Option

This option is used only if nest locations have been specified as described in Sec. 2.2.7. To do this, a value (e.g., 1, 2, 4,...) is entered to indicate the number of selected nest sites desired by the user. The grid UTM coordinates and other characteristics of these sites are required as additional input to be described later in this section.

2.2.9 Exponential Feeding Function Option (0, 1)

Entering a value of "0" makes the assumption that an animal feeds uniformly throughout its HR. An entered value of "1" assumes that an exponential feeding function related to distance from a given nest site will be used to estimate an HI around a specific nest site. This function assumes an exponential decrease in foraging as the distance from the nest site is increased within the HR of the animal as shown below (also see Equation 9e):

$$Y = EXP(-R_i/R_c), \qquad (9f)$$

where

Y = grid food utilization fraction,

R_i = distance, m, of food grid from nest site grid, and

R_c = proportionality constant, m.

2.2.10 Exponential Feeding Function Proportionality Constant (CM)

If a value of "1" was selected as described in Sec. 2.2.9 above, then the proportionality constant (CM), in meters (m), must be entered. The value reflects cumulative feeding fraction of about 66% at a distance from a nest equal to this constant.

2.2.11 Inclination Factor of HR from the E-W Axis

This input allows the user to adjust the direction of the HR of an animal along the E-W axis to align it with natural surface characteristics, such as a canyon or a river

course, consistent with foraging areas. A value of "0" leaves the alignment parallel to the E-W axis. A negative value inclines the HR in a NW-SE direction, whereas, a positive value inclines in a SW-NE direction. The tangent of the inclination angle desired is entered as the inclination factor.

2.2.12 HR Shape Factor (1, 2, 3,...)

The HR area may be shaped using the *X-axis/Y-axis* ratio to create a rectangle of desired height-to-width ratio. Shaping the HR enables the user to simulate foraging that occurs on the basis of natural topographic or habitat characteristics such as canyons or rivers. A value of "0" produces a square HR around a nest grid cell; a value of "2" produces a rectangular HR with a 2:1 ratio of length to width with the length aligned along the E-W axis. Other whole number positive values can also be entered to obtain greater ratios as appropriate. This input combines with input in Sec. 2.2.11 above to produce the desired shape and orientation for the HR around a nest site.

2.3 Input File Requirements for Input Files *inrsk.dat, mapcde.dat,* and *eeuinp.dat*

Input file requirements were briefly described in Sec. 2.2.4 with respect to terminal input options. The following is a listing of file contents, which can be entered by the user as described in Sec. 2.2. Either spaces and/or commas separate all columnar data.

Although the separate input files are described in order below, the ECORSK.5 model calls input not all at once for a given file, but as needed from all three. Additionally, the input file *eeuinp.dat* is rewound a number of times to extract information as needed. Finally, the input file *mapcde.dat* is generated from a GIS UTM coordinate file using the FORTRAN77 code CONVRT to be described in this section.

2.3.1 Input File *inrsk.dat* Description

An example of an *inrsk.dat* input file constructed for execution of ECORSK.5 for the southwestern willow flycatcher is shown in Table 1. Sections 2.3.1.1 through 2.3.1.6 describe Table 1 line by line.

2.3.1.1 Line 1 (5 columns)

column 1: number of contaminated cells in gridded area
column 2: number of E-W grids
column 3: number of N-S grids
column 4: number of random nests to be used in run
column 5: number of rows in file *eeuinp.dat* The number of rows in *eeuinp.dat* is required to separate selected nest sites from other potential sites supplied as input or generated randomly. A value of "0" may be entered for both columns 1 and 5 if *eeuinp.dat* is a complete file since ECORSK.5 will determine these quantities automatically.

2.3.1.2 Line 2 (1 column)

column 1 : name of animal simulated. The name must be bracketed by single quotation marks if entered from the terminal, otherwise without them.

2.3.1.3 Line 3 (2 columns)

column 1: type of animal (1, 2, 3, or 4) : A value of "1" is for mammals; a value

Table 1. Example of *inrsk.dat* Input File (Source: Gonzales et al., 1998b)

143.000	175.0	120.0	100.0000	11098.0
Willow flycatcher				
2	10			
0.0150000	5.000000E-02	0.0		
10.218	0.000000E+00			
1.651572E+06	1.634172E+06	1.763338E+06	1.751438E+06	

2.3.1.4 Line 4 (3 columns)

column 1: body weight of animal, kgfwt
column 2: fraction of ingested food composed of soil
column 3: equivalent sediment fraction of ingested food. A value of "0" is used if sediment uptake is not used. This parameter is used for fish-eating animals where concentrations in fish tissues and overlying sediments can be estimated to obtain this fraction (see Sec. 1.6).

2.3.1.5 Line 5 (2 columns)

column 1: area of EEU, km^2
column 2: area of HR, km^2. An entered value of "0" defaults to determination of HR by allometry in ECORSK.5 using the following relationships developed by Peters (1993):

$HR = 1.39\ BW^{1.37}$	mammal, carnivore	(10a)
$HR = 0.032\ BW$	mammal, herbivore	(10b)
$HR = 8.3\ BW^{1.37}$	avian, carnivore	(10c)
$HR = 0.026\ BW^{1.71}$	avian, herbivore	(10d)
$HR = 0.12\ BW^{0.95}$	reptiles and amphibians,	(10e)

where

HR = HR of animal, km^2, and
BW = body weight of animal, kgfwt (see Sec. 2.2.3.3, col. 1).

The corresponding HR estimates for omnivorous mammalian and avian species were estimated from scatter plots of Peters (1993) to be the mean of carnivore-herbivore types for each group.

2.3.1.6 Line 6 (4 columns)

column 1: maximum E-W UTM coordinate of gridded study area
column 2: minimum E-W UTM coordinate of gridded study area
column 3: maximum N-S UTM coordinate of gridded study area
column 4: minimum N-S UTM coordinate of gridded study area

The gridded study area includes the EEU and is the area within which HRs are established around nest sites. A unit grid cell area of 100 feet on a side is used in ECORSK.5 to build the gridded study area for HI estimations.

2.3.2 Input File *eeuinp.dat* Description

The GIS/ARC/INFO-derived *eeuinp.dat* database input file is structured line by line with 12-column input. As shown in Table 2, each line of information in *eeuinp.dat* contains the following information:

column 1: number of COCs in specific grid cell
column 2: COC concentration, mg/kg, (or, pCi/gdwt soil, if COC is a radionuclide)
column 3: background COC concentration, mg/kg or pCi/gdwt soil
column 4: E-W UTM coordinates for grid cell

column 5: N-S UTM coordinates for grid cell
column 6: COC TRV, mg/kg/day or pCi/g (ESAL for radionuclide)as described above
column 7: enhancement/devaluation factor for feeding in any one grid cell
column 8: TRV adjustment factor
column 9: area of grid cell, km^2
column 10: weighted BAF or BMF of specified COC
column 11: x, y location of grid cell surrounded by single quotation marks
column 12: name of contaminant (surrounded by single quotation marks)

Data included in columns 1, 4, 5, 7, 9, and 11 are repeated for each COC present in a given grid cell; the other columns generally have different values for each COC. The process is repeated for each grid cell in the database. Since input from the file *eeuinp.dat* is taken from a specified number of columns at a time, the file must be rewound after each data extraction to obtain the next set of data as will be shown below for required input. If the file is being created via terminal interaction, then values must be repeated as the case may be for each COC of every grid cell in any given HR. All information entered from the terminal or from *eeuinp.dat* file extraction is stored in the output file *gis.dat* for verification purposes and input error detection. *Gis.dat* is not in same format as *eeuinp.dat* used for input and can not be used as a substitute file as described for *entrsk.dat* in Sec. 2.3.1 above. ECORSK.5 also has some input error diagnostics included as part of the code. The detection of an input error from terminal input will result in a repetition of the input instruction until the error is corrected. Finally, an end-of-file (EOF) detection in execution of ECORSK.5 will result in a change to the terminal input. The user then has the option of reverting back to file input status for the next set of input or remaining in terminal mode. ECORSK.5 will query the user for this purpose.

2.3.2.1 Line 1 (1 column)

column 1: number of contaminants in a grid cell (column 1 in Sec. 2.3.2 above). This value is repeated for each COC present. As an example: if there are 10 COCs present in a given grid cell, then 10 input lines with the value (10) are entered for the specific grid cell in question from the terminal or from 10 lines of input present in *eeuinp.dat.* Information for all grid cells in the database is entered in this manner before rewinding *eeuinp.dat* (if file input has been specified).

2.3.2.2 Line 2 (1 column)

column 1: location of grid cell surrounded by single quotes.. '67-31'...etc. (column 11 in Sec. 2.3.2). This input is repeated for each contaminant present in a specific grid cell. Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.2.3 Line 3 (1 column)

column 1: the name of contaminant surrounded by single quotes, e.g., 'Mercury' (column 12 in Sec. 2.3.2). Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.2.4 Line 4 (3 columns)

column 1: contaminant concentration in soil, mg/kgdwt, or pCi/gdwt for radionuclides (column 2 in Sec. 2.3.2).
column 2: background concentration of contaminant, mg/kgdwt or pCi/gdwt for

Table 2. Example of Partial *eeuinp.dat* File Constructed for Executing ECORSK.5 for the American Peregrine Falcon (Source: Gallegos et al., 1997b).

41	61879	266	1626498.00	1783255.00	109.7	1.00	1.00	9.29e-04	0.00	'119-83'	'Aluminum'
41	5.00	0.50	1626498.00	1783255.00	1.15	1.00	1.00	9.29e-04	0.00	'119-83'	'Antimony'
41	1.84	6.99	1626498.00	1783255.00	1.15	1.00	1.00	9.29e-04	0.00	'119-83'	'Arsenic'
41	331.5	263	1626498.00	1783255.00	20.79	1.00	1.00	9.29e-04	0.00	'119-83'	'Barium'
41	2.25	1.41	1626498.00	1783255.00	0.54	1.00	1.00	9.29e-04	0.00	'119-83'	'Beryllium'
41	0.50	1.40	1626498.00	1783255.00	1.45	1.00	1.00	9.29e-04	0.00	'119-83'	'Cadmium'
41	3920.	4030	1626498.00	1783255.00	24.00	1.00	1.00	9.29e-04	0.00	'119-83'	'Calcium'
41	11.00	19.30	1626498.00	1783255.00	3.80	1.00	1.00	9.29e-04	0.00	'119-83'	'Chromium'
41	8.25	31.00	1626498.00	1783255.00	0.00	1.00	1.00	9.29e-04	0.00	'119-83'	'Cobalt'
41	2.50	30.70	1626498.00	1783255.00	46.97	1.00	1.00	9.29e-04	0.00	'119-83'	'Copper'
41	0.12	0.00	1626498.00	1783255.00	0.40	1.00	1.00	9.29e-04	0.00	'119-83'	'Dinitrobenzene [1,3-]'
41	0.12	0.00	1626498.00	1783255.00	0.20	1.00	1.00	9.29e-04	0.00	'119-83'	'Dinitrotoluene [2,4-]'
41	0.13	0.00	1626498.00	1783255.00	0.00	1.00	1.00	9.29e-04	0.00	'119-83'	'Dinitrotoluene [2,6-]'
41	1.11	0.00	1626498.00	1783255.00	50.00	1.00	1.00	9.29e-04	0.00	'119-83'	'HMX'
41	15171	18100	1626498.00	1783255.00	0.00	1.00	1.00	9.29e-04	0.00	'119-83'	'Iron'
41	72.25	28.40	1626498.00	1783255.00	1.12	1.00	1.00	9.29e-04	0.00	'119-83'	'Lead'
41	25.75	0.00	1626498.00	1783255.00	150	1.00	1.00	9.29e-04	0.00	'119-83'	'Lithium'
41	1867	3460	1626498.00	1783255.00	1000	1.00	1.00	9.29e-04	0.00	'119-83'	'Magnesium'
41	561	1000	1626498.00	1783255.00	9.14	1.00	1.00	9.29e-04	0.00	'119-83'	'Manganese'
41	1.75	0.00	1626498.00	1783255.00	0.28	1.00	1.00	9.29e-04	0.00	'119-83'	'Molybdenum'
41	5.50	12.20	1626498.00	1783255.00	0.67	1.00	1.00	9.29e-04	0.00	'119-83'	'Nickel'

radionuclides (column 3 in Sec. 2.3.2).

column 3: area of grid cell, km^2 (column 9 in Sec.2.3.2)

.

Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.2.5 Line 5 (1 column)

column 1: enhancement/devalue fraction for a given grid cell, which is based on food availability and/or other factors (column 7 in Sec. 2.3.2). Information for all grid cells is entered as in Sec. 2.3.2.1 above. Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.2.6 Line 6 (1 column)

column 1: to TRV, mg/kg/day, or, pCi/g , (ESAL) for the specific COC to the specific animal tested (column 6 in Sec. 2.3.3). Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.2.7 Line 7 (1 column)

column 1: TRV adjustment factor for a given COC (column 8 in Sec. 2.3.2 above). Information for all grid cells is entered as in Sec. 2.3.2.1 above.

2.3.3 Input File *mapcde.dat* Description and Generation Using CONVRT

The input file *mapcde.dat* (renamed from a CONVRT output file called *mapper.dat*) is generated from an ARC/INFO database file called *grid.dat* using the FORTRAN77 code CONVRT. The file identification numbers are

grid.dat [INPUT], unit = 5
mapper.dat [OUTPUT], unit = 6
mapplt.dat. [OUTPUT], unit = 7

The latter two files must be entered as dummy files initially (see Sec. 2.1), and *grid.dat* must also be entered as such if terminal input is to be used.

CONVRT accepts the input data from *grid.dat* and generates a three-dimensional

surface data composed of the following elements:

- cell x-coordinate (integer)
- cell y-coordinate (integer)
- cell value (integer)

As shown in Table 3, the cell values are used to identify the specific characteristic of each cell where

- a value of "0" identifies a cell within the grid network that is not within the EEU and is not used in making HI estimates because it is outside the HR of the animal in question,
- a value of "1" identifies a cell within the EEU, which will be included in making HI estimates for the animal in question,
- a value of "98" identifies a cell that is part of a river grid within the EEU (See Sec. 1.6 for more details on the use of this information),
- a value of "99" identifies potential nest sites within the nesting habitat, which is used to obtain HI estimates, and
- the x, y coordinate values are sorted starting with the top row (north), entering from west to east for each line of input. In addition to the output file *mapper.dat* generated from CONVRT output, another output file *mapplt.dat* is generated which can be used to generate a three-dimensional surface plot of the gridded surface used in the study using the auxiliary code called PLTRSK to be described later in this report.

The use of CONVRT requires that the files *grid.dat*, *mapper.dat*, and *mapplt.dat* be present, with the latter two files in dummy form initially as described earlier for files required by ECORSK.5 (Sec. 2.1). If the user is creating an input file, then the *grid.dat* input file required for CONVRT execution may be created directly for use as described below.

2.3.3.1 Line 1 (2 columns)

column 1: number of rows in gridded area
column 2: number of columns in gridded area
The current maximum number of rows and columns are 600 by 600, which is set by the parameter statement in ECORSK.5. Row or column data exceeding these maxima cannot be entered without recompiling ECORSK.5 with appropriate changes of the parameter statement. Also, the size of an individual grid cell is set 100 feet on a side by the current version of ECORSK.5.

2.3.3.2 Line 2 (blank row)

2.3.3.3 Line 3 (blank row)

2.3.3.4 Line 4 (5 columns)

column 1: y-cell index number (integer). The initial address must be the NW corner of the gridded area (1).
column 2: x-cell index number (integer). The initial address must be the NW corner of the gridded area (1).

Entering all columns (x-cell data), before incrementing the y-cell index (proceeding from the NW corner to the NE corner before incrementing the N-S direction by one) enters the remaining cell indices. Input proceeds in this fashion until the cell in the SE corner is entered.

column 3: N-S UTM coordinate for the cell (x, y)
column 4: W-E UTM coordinate for the cell (x, y)

Table 3. Example of Partial *mapcde.dat* File Used to Execute ECORSK.5 for an Assessment of the Mexican Spotted Owl (Source: Gallegos et al., 1998a).

```
0  0  0  0  0  1  1  1  1  1  1  1  1  99 99 99 99 99 1  1  1  1
   1  1  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 99 99
   1  1  1  1  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 99 99
   99 99 99 99 1  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 99
   99 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 99 99
   99 99 99 99 99 99 99 1  1  1  1  1  1  99 99 99 99 99 99 99 99
   99 99 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   0  0  0  0  0  0  0  0  0  0  0  0  0
0  0  0  0  0  1  1  1  1  1  1  1  1  99 99 99 99 99 99 99 99 99
   99 99 99 99 99 99 99 99 99 99 1  1  1  99 99 99 99 99 99 99 99
   99 99 99 99 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
   0  0  0  0  0  0
```

column 5: cell value, integer (See Sec. 2.3.3 above)

2.3.4 Input File Description and Output Generation Using PLTRSK

The FORTRAN77 PLTRSK code is designed to plot two- and three-dimensional GIS data derived from ARC/INFO and HQ output from ECORSK.5. The three-dimensional data are graphed as either two- or three-dimensional contours, and the code has a built-in option for superimposing three-dimensional graphics one upon the other. Figure 3 is an example of the plotting capabilities of PLTRSK where HQ results have been superimposed on an EEU. In addition to required terminal input described below, the following files must be present as input or dummy files before execution can proceed:

inplt1.dat [INPUT], unit = 7
entplt1.dat [OUTPUT], unit = 6
inplt2.dat [INPUT], unit = 8
entplt2.dat [OUTPUT], unit = 9
inplt3.dat [INPUT], unit = 10
entplt3.dat [OUTPUT], unit = 11

Dummy files are created (when not present) by entering one line of numeric input such as 1.0 and saving as such (see Sec. 2.1). The use of these files will be described below.

2.3.4.1 Description of Terminal Input to PLTRSK

2.3.4.1.1 Line 1 (1 column)

column 1: number of graphs being processed. A maximum of eight graphs are possible. The output of these graphs

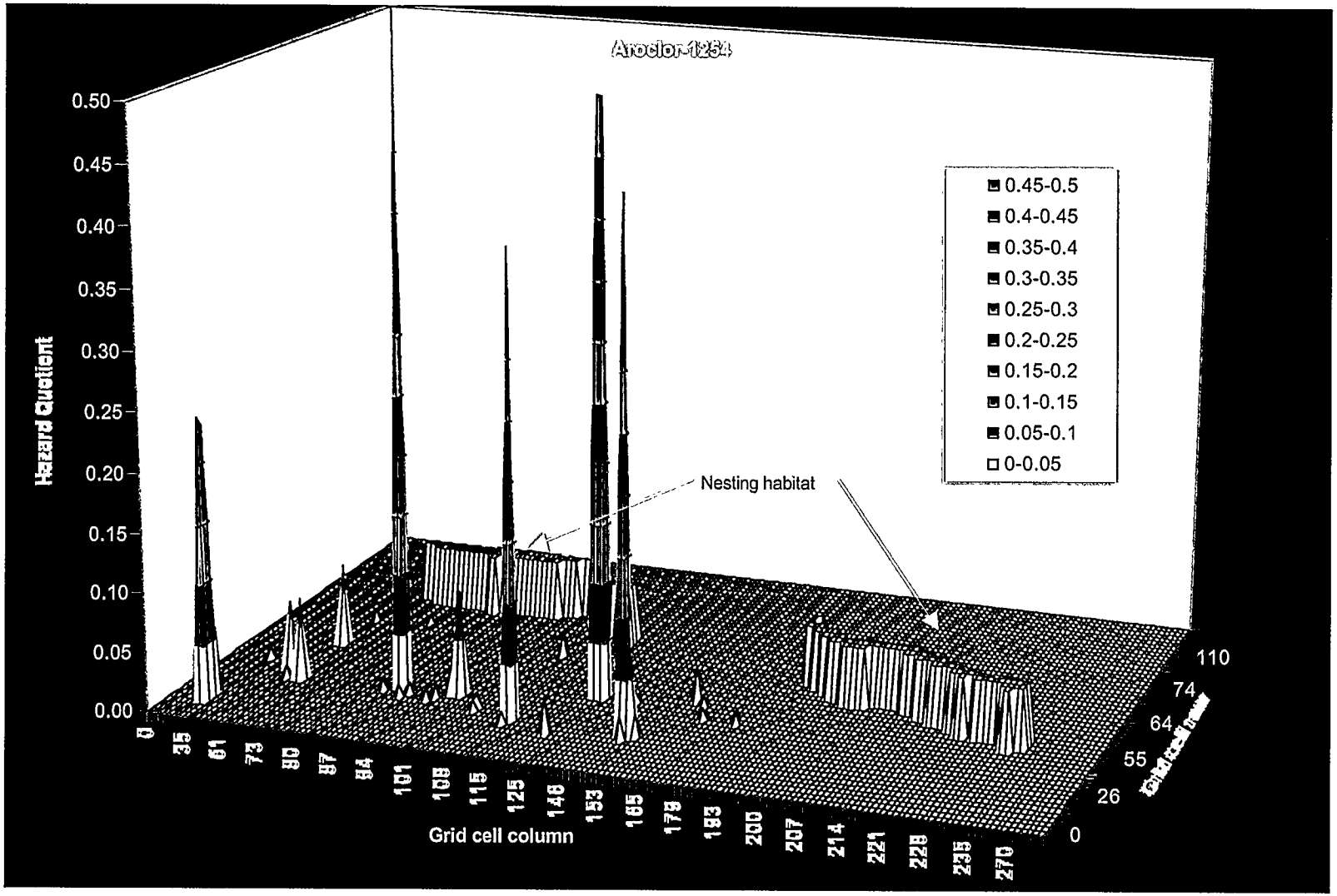

Figure 3. Example of the plotting capabilities of PLTRSK where HQ results have been superimposed on an EEU.

is HP-GL files labeled as *plot1.plt*, *plot2.plt*, *plot3.plt*...*plot8.plt*. Separate plot information will be requested for each plot considered in the run.

2.3.4.1.2 Line 2 (1 column)

column 1: Is existing input file *inplt1.dat* present? A value of "1" indicates yes; a value of "0" indicates no. This file refers to input to be described in Sec. 2.3.4.2 below. If input must be entered from the terminal, then dummy files *inplt1.dat* and *entplt1.dat* must be present for this purpose. After the run, the file *entplt1.dat* can be saved in a unique subdirectory and/or given a special file name. This is necessary because *entplt1.dat* will be overwritten when the next execution of ECORSK.5 occurs.

2.3.4.1.3 Line 3 (1 to 8 columns)

column 1: the number of variables plotted on the first graph.
column 2: the number of variables plotted on the second graph.
column n: the number of variables plotted on the *nth* graph, where n = the number of graphs to be generated given in Sec. 2.3.4.1.1.

This input is most commonly used for two-dimensional graphs but can have some utility with three-dimensional graphs if the z-axes are properly scaled so that one plot lies above the other and does not erase it. A maximum of eight variables per plot is allowed. Separate information will be requested for each dependent variable in each plot.

2.3.4.1.4 Line 4 (1 to 8 columns)

column 1: A value of "0" specifies a border for axes; a value of "1" specifies a regular axes for the first graph.
column 2: A value of "0" specifies a border for axes; a value of "1" specifies a regular axes for the second graph.
column n: A value of "0" specifies a border for axes; a value of "1" specifies a regular axes for the n*th* graph, where n = the number of graphs to be generated as described in Sec. 2.3.4.1.1.

2.3.4.1.5 Line 5 (1 to 8 columns)

column 1: x-coordinate for the legend. A value of "0" is entered when a legend is not specified for the first graph.
column 2: x-coordinate for the legend. A value of "0" is entered when a legend is not specified for the second graph.
column n: x-coordinate for the legend. A value of "0" is entered when a legend is not specified for the n*th* graph, where n = the number of graphs to be generated described in Sec.2.3.4.1.1.

2.3.4.1.6 6 (1 to 8 columns)

column 1: y-coordinate for the legend. A value of "0" is entered when a legend is not specified for the first graph.
column 2: y-coordinate for the legend. A value of "0" is entered when a legend is not specified for the second graph.
column n: y-coordinate for the legend. A value of "0" is entered when a legend is not specified for the n*th* graph, where n = the number of graphs to be generated described in Sec. 2.3.4.1.1.

An example of a well-placed legend when a border axis is used is x = 64, y = 67, which places the legend on the upper right

hand part of the plot. Non-zero choices above will signal a legend request below.

2.3.4.1.7 Line 7 (1 to 8 columns)

column 1: two-dimensional or three-dimensional plot option: a value of "2" selects for a two-dimensional plot; a value of "3" selects for a three-dimensional plot for the first graph.
column 2: two-dimensional or three-dimensional plot option: a value of "2" selects for a two-dimensional plot; a value of "3" selects for a three-dimensional plot for the second graph.
column n: two-dimensional or three-dimensional plot option: a value of "2" selects for a two-dimensional plot; a value of "3" selects for a three-dimensional plot for the n*th* graph, where n = the number of graphs to be generated as described in Sec. 2.3.4.1.1.

2.3.4.1.8 Line 8 (n columns)

column 1: two-dimensional or three-dimensional contour option for three-dimensional plots only. A value of "2" specifies a two-dimensional contour plot; a value of "3" specifies a three-dimensional contour plot; a value of "0" specifies a non-contour three-dimensional plot, or when a two-dimensional plot has been specified in Sec. 2.3.4.1.7 above for the first graph.
column 2: two-dimensional or three-dimensional contour option for three-dimensional plots only. A value of "2" specifies a two-dimensional contour plot; a value of "3" specifies a three-dimensional contour plot; a value of "0" specifies a non-contour three-dimensional plot, or when a two-dimensional plot has been specified in Sec. 2.3.4.1.7 above for the second graph.
column n: two-dimensional or three-dimensional contour option for three-dimensional plots only. A value of "2" specifies a two-dimensional contour plot; a value of "3" specifies a three-dimensional contour plot; a value of "0" specifies a non-contour three-dimensional plot, or when a two-dimensional plot has been specified in Sec. 2.3.4.1.7 above for the *nth* graph, where n = the number of graphs to be generated as specified in Sec. 2.3.4.1.1.

2.3.4.1.9 Line 9 (1 to 8 columns)

column 1: the number of contour intervals required for the first graph. A maximum of 10 is presently set by the code.
column 2: the number of contour intervals required for the second graph. A maximum of 10 is presently set by the code.
column n: the number of contour intervals required for the n*th* graph. A maximum of 10 is presently set by the code, where n = the number of graphs to be generated as specified in Sec. 2.3.4.1.1.

A value of "0" is entered when contouring is not desired or when the graph is two-dimensional.

2.3.4.1.10 Sub-lines 1 through *x*

Upper contour values are specified for those graphs 1 through x ($x \leq 8$) which are to be contoured. A rule of thumb is to add a value of (0.001) to any contour interval such as 1.001, 10.001 ..etc., to capture grid, EEU, and nest site information as separate layers. ECORSK.5 automatically assigns grid values "0", EEU values "1", and "10" for independent plots; a value of "2" is assigned to superimposed plots. Some

experimentation is helpful to attain the desired separation of grid information.

2.3.4.1.10.1 Sub-line 1 (1 column)

column 1: upper contour value for the first graph.

2.3.4.1.10.2 Sub-line 2 (1 column)

column 1: upper contour value for the second graph.

2.3.4.1.10.*x* Sub-line *x* (1 column)

column 1: upper contour value for the *xth* graph, $x \leq 8$.

The total number of sub-lines of input will vary from 0 to 8 depending on the number of contoured graphs specified in 2.3.4.1.8 above.

2.3.4.1.11 Line 11 (1 to 8 columns)

This line specifies the number of x, y or x, y, z observations required for data stored in *inplt2.dat*. This is the only graph information for x, y plots and for the reference file when using a superimposed file stored in *inplt3.dat*. Input specifications for these files are presented later in this report.

column 1: number of observations for the first graph.
column 2: number of observations for the second graph.
column n: number of observations for the *nth* graph, where n = the number of graphs to be generated as specified in Sec. 2.3.4.1.1.

2.3.4.1.12 Line 12 (1 to 8 columns)

column 1: Option to omit zero value observations of the dependent variable (y, z) from the dataset for the first graph. A value of "0" preserves this data; a value of "1" removes this data.
column 2: Option to omit zero value observations of the dependent variable (y, z) from the dataset for the second graph. A value of "0" preserves this data; a value of "1" removes this data.
column n: Option to omit zero value observations of the dependent variable (y, z) from the data set for the n*th* graph, where n = the number of graphs to be generated given in Sec. 2.3.4.1.1. A value of "0" preserves this data; a value of "1" removes this data.

2.3.4.1.13 Line 13 (1 to 8 columns)

This input determines whether other x, y, z data will be superimposed on the current plot. Data of the x, y, z type are stored in *inplt2.dat* or must be created (user is prompted whether data is available or terminal input is required). Other data of the x, y, z type can be stored in *inplt3.dat* or must be created (user is prompted whether data is available or terminal input is required) for superimposing on *inplt2.dat* data if requested by the user. As with *inplt1.dat*, terminal created input is stored in file *entplt2.dat* and *entplt3.dat* for conversion to *inplt2.dat* and *inplt3.dat* data, respectively, to be used in future executions. (Note that files are overwritten each time ECORSK.5 is executed, therefore if they have information that will be used at a later time, they should be moved to a special subdirectory, as described for *entplt1.dat*. If a value of "0" is entered, then data in the file *inplt2.dat* is all that is required for the run.)

column 1: superimposition option. A value of "0" skips the option; a value of "1" selects the option for the first graph.
column 2: superimposition option. A value of "0" skips the option; a value of "1" selects the option for the second graph.
column n: superimposition option. A value of "0" skips the option; a value of "1" selects the option for the *nth* graph, where n = the number of graphs to be generated as described in Sec.2.3.4.1.1.

2.3.4.1.14 Sub-lines 1 through *x*

A scaling factor is required for superimposed data. This is usually done to lift the data above the EEU- and nest site-entered values on the plots and requires user judgement and experimentation to produce good plots. A value of 10 is added to each superimposed z-datum in addition to the scaling factor to assure differentiation from grid, EEU, and nest data. A note should be made in the legend or elsewhere to account for data scaling. If superimposition is not requested, then the scaling parameter is ignored for a given graph.

2.3.4.1.14.1 Sub-line 1 (1 column)

column 1: Scaling parameter for the first graph.

2.3.4.1.14.2 Sub-line 2 (1 column)

column 1: Scaling parameter for the second graph.

2.3.4.1.14.*x* Sub-line *x* (1 column)

column 1: Scaling parameter for the *xth* graph, $x \leq 8$.

2.3.4.2 Description of Input File *inplt1.dat* Required for PLTRSK Execution

This file can be created during or before PLTRSK execution. An index number is used for re-entering data when the user detects an error and wishes to re-enter the entire file. However, the user is also queried during terminal input whether the current line of input is accurate or is to be re-entered.

2.3.4.2.1 Line 1 (1 column)

column 1: The index number 191919 is requested as input.

2.3.4.2.2 Sub-lines 1 through *n* ($n \leq 8$)

2.3.4.2.2.1 Sub-line 1 (3 to 4 columns)

column 1: number of columns (letters) in the x-axis label.
column 2: number of columns (letters) in the y-axis label.
column 3: number of columns (letters) in the title label (two-dimensional graph) or number of columns (letters) in the z-axis label (three-dimensional graph).
column 4: Number of columns (letters) in the title label (three-dimensional graph only).

Extra spaces are added for centering purposes as necessary. Up to 40 columns for each label may be used inclusive of blanks used for centering purposes.

2.3.4.2.2.2 Sub-sub-lines 1 through *n* ($n \leq 8$)

Each graph requested requires specific plotting instructions for all independent variables in each plot (two-dimensional only). For three-dimensional graphics, only one independent variable (z-

value) is allowed. Hence, only one column of input is required for graphs of this type when the number of independent variables is specified.

2.3.4.2.2.1 Sub-sub-line 1 (1 to 8 columns)

column 1: type of marker desired for the first independent variable of the first graph. A value of "0" specifies no marker; a value of "1" specifies digits; a value of "3" specifies letters; and a value of "4" specifies symbols. For a three-dimensional graph, a value of "0" is used.

column 2: type of marker desired for the second independent variable of the first graph. A value of "0" specifies no marker; a value of "1" specifies digits; a value of "3" specifies letters; and a value of "4" specifies symbols. This column is not used for three-dimensional graphics.

column *n*: type of marker desired for the *nth* independent variable of the first graph. A value of "0" specifies no marker; a value of "1" specifies digits; a value of "3" specifies letters; and a value of "4" specifies symbols. This column is not used for three-dimensional graphics.

2.3.4.2.2.3 Sub-line 3 (1 column)

column 1: color graphics requested: A 'y' specifies yes; an 'n' specifies no. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e.,'y' or 'n' as shown or without quotes if the input file *inplt1.dat* is used.

2.3.4.2.2.4 Sub-line 4 (1 column)

column 1: Legend requested: A 'y' specifies yes; a 'n' specifies no. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'y' or 'n' as shown or without quotes if the input file *inplt1.dat* is used.

2.3.4.2.2.5 Sub-line 5 (1 column)

column 1: $\log_{10}$ of y-values request. A 'y' specifies yes; a 'n' specifies no. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e.,'y' or 'n' as shown or without quotes if the input file *inplt1.dat* is used.

2.3.4.2.2.6 Sub-line 6 (1 column)

column 1: $\log_{10}$ of x-values request. A 'y' specifies yes; a 'n' specifies no. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e.,'y' or 'n' as shown or without quotes if the input file *inplt1.dat* is used.

2.3.4.2.2.7 Sub-line 7 (1 column)

column 1: $\log_{10}$ of z-values request. A 'y' specifies yes; a 'n' specifies no. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'y' or 'n' as shown or without quotes if the input file *inplt1.dat* is used. Two-dimensional graphics ignore this request.

2.3.4.2.2.8 Sub-line 8 (label, 1 to 40 columns)

columns 1 to 40: Title for x-axis. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'x-axis,' otherwise without quotes if file input is used.

2.3.4.2.2.9 Sub-line 9 (label, 1 to 40 columns)

columns 1 to 40: Title for y-axis. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'y-axis,' otherwise without quotes if file input is used.

2.3.4.2.2.10 Sub-line 10 (label, 1 to 40 columns)

columns 1 to 40: Title for z-axis. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'z-axis,' otherwise without quotes if file input is used. For three-dimensional plots only, otherwise ignored.

2.3.4.2.2.11 Sub-line 11 (label, 1 to 40 columns)

columns 1 to 40: Graph title. If entering data from a terminal, all alphanumeric data must be entered with single quotes, i.e., 'title' otherwise without quotes if file input
is used.

2.3.4.2.2.12 Sub-sub-lines 1 through *n*, ($n \leq 8$)

2.3.4.2.2.12.1 Sub-line 1 (label, 1 to 8 columns)

columns (1 to 8): title for y-variables (two-dimensional) or contour interval (three-dimensional) for legend of first variable of the first graph.

2.3.4.2.2.12.2 Sub-sub-line 1 (label, 1 to 8 columns)

columns (1-8): title for y-variables (two-dimensional) or contour interval (three-dimensional) for legend of second variable of the first graph.

2.3.4.2.2.12.*n* Sub-sub-line 1 (label, 1 to 8 columns)

columns (1-8): title for y-variables (two-dimensional) or contour interval (three-dimensional) for legend of *nth* variable of the first graph ($n \leq 8$).

2.3.4.2.2.13 Sub-line 13 (2 columns)

column 1: minimum of x-values. The minimum x-value will be determined by ECORSK.5 if the value (-111) is entered.
column 2: maximum of x-values. The maximum x-value will be determined by ECORSK.5 if the value (-111) is entered.

2.3.4.2.2.14 Sub-line 14 (2 columns)

column 1: minimum of y-values. The minimum y-value will be determined by ECORSK.5 if the value (-111) is entered.
column 2: maximum of y-values. The maximum y-value will be determined by ECORSK.5 if the value (-111) is entered.

2.3.4.2.2.15 Sub-line 15 (2 columns)

column 1: minimum of z-values. The minimum z-value will be determined by ECORSK.5 if the value (-111) is entered. Instruction is ignored for two-dimensional graphs.

Input is repeated starting at Sec. 2.3.4.2.2 for all n graphs being generated ($n \leq 8$).

2.3.4.3 Description of Input File *inplt2.dat* Required for PLTRSK Execution

This file can be created with or without PLTRSK execution. The file *entplt2.dat* created during the run can be substituted for *inplt2.dat* after renaming. Remember to re-create the dummy *entplt2.dat* when the latter is renamed as described. This input is ignored for two-dimensional graphics.

column 1: x-value
column 2: y-value
column 3: z-value

The three-column input is repeated until all observations have been entered. A maximum of 52,000 observations is allowed. The total number of observations for all graphs is specified in Sec. 2.3.4.1.11 above. Files *gridxy.dat*, *habit.dat*, and other files generated by ECORSK.5 can be used directly if renamed to *inplt2.dat*. A description of these files and their use has been discussed in Sec. 2.1 above. These files contain up to six lines of description and/or six blank lines that should be removed before renaming to *inplt2.dat*.

2.3.4.4 Description of Input File *inplt3.dat* Required for PLTRSK Execution

This file can be created with or without PLTRSK execution. This file is not used for two-dimensional graphics, but a dummy file must be present. The file *entplt3.dat* created during the file input can be substituted for *inplt3.dat* (three-dimensional) after renaming. Remember to create the dummy file *entplt3.dat* after renaming it to *inplt3.dat*. The number of observations in the files *hq.dat*, *hqpo.dat*, *hqpco.dat*, and other files generated by ECORSK.5 and SELECT can be used directly if renamed to *inplt3.dat*. A description of these files and their use is discussed in Sec. 2.1 and in the description of input for SELECT in the next section. This file contains up to six lines of description and/or six blank lines which should be removed before renaming to *inplt3.plt*. Some experimentation with this code may be necessary to optimize graphics quality.

column 1: x-value
column 2: y-value
column 3: z-value

The three-column input is repeated until all observations have been entered. A maximum of 52,000 observations is allowed.

2.3.5 HQs (*hqp.dat* and *hqpc.dat*)

ECORSK.5 generates HQ data of two types that can be used for plotting as described in the next section. The two types are: (1) in the file *hqp.dat,* an HQ for all COCs totaled is reported for each grid cell in the HR of a given animal; (2) in the file *hqpc.dat,* ECORSK.5 reports an HQ by contaminant for all grid cells totaled within a given HR. As examples, Table 4 (a and b) presents portions of *hqp.dat* and *hqpc.dat* for an assessment of the bald eagle and the southwestern willow flycatcher.

2.3.6 SELECT Code

2.3.6.1 Input File Description and Output Generation

The SELECT code selects pHQ data obtained from ECORSK.5 analyses of different animal types living in a given EEU. The following files must be present for SELECT to execute:

Table 4. Examples of Partial Output Files (a) *hqp.dat* and (b) *hqpc.dat* Generated by ECORSK.5 for an Assessment of the Southwestern Willow Flycatcher (Source: Gonzales et al., 1998b).

(a) Columns 1 and 2 = x, y coordinate of the grid cell contributing the HQ to the nest site identified in columns 5 and 6; Col. 3 = partial HQ; Col. 4 = Nest index no.; Col. 5, 6 = x, y coordinate of nest; Col. 7 = parameter.

68	63	0.253224	23	69	60	HQP
69	63	0.270911	23	69	60	HQP
70	63	0.284314	23	69	60	HQP
78	63	0.00E+00	23	69	60	HQP
121	64	0.00E+00	23	69	60	HQP
23	64	0.00E+00	23	69	60	HQP
62	64	0.00E+00	23	69	60	HQP
68	64	0.281765	23	69	60	HQP
121	65	0.00E+00	23	69	60	HQP
19	65	0.00E+00	23	69	60	HQP
60	65	0.00E+00	23	69	60	HQP

(b) Column 1 and 2 = x, y coordinate of nest; Column 3 = partial HQ for a nest site due to the particular COC listed in column 6; Column 4 = COC index; Column 5 = number of observations for the particular COC; Column 7 = nest index number.

71	60	1.512198E-04	1	3.00000	Trinitrotoluene [2,4]	9	HQPC
71	60	3.780495E-04	2	3.00000	Dinitrotoluene [2,4-]	9	HQPC
71	60	1.008132E-03	3	3.00000	RDX	9	HQPC
71	60	0.000000E+00	4	3.00000	Amino-2,6-dinitrotoluene	9	HQPC
71	60	1.298711E-05	5	3.00000	HMX	9	HQPC
71	60	0.000000E+00	6	3.00000	Amino-4,6-dinitrotol	9	HQPC
71	60	0.000000E+00	7	3.00000	Tetryl (methyl-2,4,6	9	HQPC
71	60	0.000000E+00	8	3.00000	Dinitrotoluene [2,6-]	9	HQPC
71	60	0.000000E+00	9	3.00000	Nitrotoluene[2-]	9	HQPC
71	60	1.647274E-05	10	3.00000	Nitrobenzene	9	HQPC
71	60	3.912277E-05	11	3.00000	m-Nitrotoluene	9	HQPC

inplt1.dat [INPUT], unit = 7
hqp.dat [INPUT], unit = 8
hqpc.dat [INPUT], unit = 5
hqpo.dat [OUTPUT], unit = 7
hqpco.dat [OUTPUT], unit = 6

Either old files of the latter two must be present, or the user needs to create dummy files using a DOS editor if they are not already present. The first two files are generated by ECORSK.5. An error will appear if any files are missing. The error message shows which file (number) is missing.

An example of using SELECT to select data for specified nest sites from the *hqpc.dat* file for the purpose of plotting is as follows:

After beginning execution, it is only necessary to

- select a value of "1" as the choice for first request and
- specify x and y coordinates of the specific nest site for next request 220, 207, etc. separated by a comma or blank space.

The resulting output is stored in the file *hqpo.dat* which can be used in plotting data. The specific nest site for which the user wants contaminant-specific HQs may be obtained by viewing the *hqp.dat* file and noting the last two columns for x-y coordinates, respectively. Please refer to Sec. 2.3.4 for plotting data using PLTRSK.

2.3.6.2 Selection of Data from *hqpc.dat*

As mentioned above, the second type of partial data refers to HQs that have been estimated by contaminant for all nest sites in the analysis. The file *hqpc.dat,* generated by ECORSK.5, contains this information. To obtain contaminant-specific data over all nest sites during execution, the following procedure is used:

- select "2" as the choice for first request and
- specify the contaminant name preceded by a blank space, e.g., Copper.

The selection is case sensitive and must correspond exactly to the way in which the contaminant was entered for processing in ECORSK.5. The file *hqpco.dat* generated by ECORSK.5 contains the selected information. Please refer to Sec. 2.3.4 for plotting of data using PLTRSK.

3.0 Execution of FORTRAN 77 Codes

ECORSK.5 and supporting codes CONVRT, PLTRSK, and SELECT are executed by the commands

- RUN77 ECORSK.5
- RUN77 CONVRT
- RUN77 PLTRSK
- RUN77 SELECT

Diagnostic information will be provided if errors in input, missing input, or parameterization errors are present during execution.

4.0 ECORSK.5 Operation

ECORSK.5 is used to estimate HQs for a specific animal from COCs present in a given EEU, which is gridded into 100- by 100-ft cells. Any number of grid cells may be specified including areas that are free of contamination. HIs are calculated when HQs for each grid cell within a HR are summed. After all input has been entered for execution of ECORSK.5 as described for this model in Sec. 2.1, ECORSK.5 transforms and integrates contaminant data stored in LANL's FIMAD with GIS/ARC/INFO and the various data and graphing subroutines of ECORSK.5 (Figure 1). This section will describe those operations that are used by the ECORSK.5 model to accomplish this task exclusive of those quantitative relationships that have been described in Sec. 1.0.

4.1 Initial Diagnostic Output from ECORSK.5

The following output will be printed on the terminal for inspection by the user:

- the number of data points in the *eeuinp.dat* input file,
- the number of grid cells or sites in the EEU with COCs present,
- the maximum number of COCs that the current version of ECORSK.5 allows,
- the number of selected sites that the user has identified as potential nest sites,
- the number of selected lines of data that the user has identified as potential nest sites,

- the number of different COCs identified in the *eeuinp.dat* input file, and
- the total number of different contaminants currently allowed by ECORSK.5.

The user should make sure that the input fits into the parameterized database arrays before proceeding. Also, some data entry errors are also printed on the terminal when they are detected.

4.2 Radionuclides Included in ECORSK.5 for HQ Determination

The following radionuclides are included in ECORSK.5 for HQ determination using the LANL ESAL method:

Plutonium-239	Technetium
Americium-241	Potassium-40
Thorium-232	Ruthenium-106
Uranium-238	Iodine-12
Cobalt-60	Strontium-90
Cobalt-57	Thorium-239
Radium-228	Uranium-235
Manganese-54	Cesium-134
Plutonium-238	Cerium-144
Thorium-228	Radium-226
Uranium-234	Sodium-22
Cesium-137	

Other radionuclides included in *eeuinp.dat* will be ignored by the current version fo the model, however, a compiled version (source code) of ECORSK.5 can be recompiled to include additional redionuclides. ECORSK.5 test for the radionuclide COCs above and designates the use of Eq.8 in Section 1.5.

4.3 Bioaccumulation and Biomagnification Factors in ECORSK.5

The 12th field of *eeuinp.dat* is used for BAFs and BMFs. ECORSK.5 treats BAFs and BMFs as multipliers.

4.4 Establishment of Cell x, y-Coordinates from UTM Coordinates

Coordinates for each cell in the EEU gridded area are established and centered within each cell as follows:

$$XCRD(n) = XCRD(n-1)+XDIST / NX \quad (11a)$$
$$YCRD(n) = YCRD(n-1)+YDIST / NY \quad (11b)$$
$$XCRD(1) = (EUEWMN+ 0.5\ XDIST / NX) \quad (11c)$$
$$YCRD(1) = (EUNSTMN+ 0.5*YDIST / NY), \quad (11d)$$

and

$$XDIST = EUNSTMX-EUNSTMN \quad (11e)$$
$$YDIST = EUEWMX-EUEWMN \quad (11f)$$

where

XCRD(n) = cell-centered x-coordinate for the *nth* grid cell, meters,

YCRD(n) = cell-centered y-coordinate for the *nth* grid cell, meters,

NX = number of cells in the E-W direction,

NY = number of cells in the N-S direction,

EUEWMN = minimum value of UTM coordinates in the E-W direction, meters,

EUNSTMN = minimum value of UTM coordinates in the N-S direction, meters,

EUEWMX = maximum value of UTM coordinates in the E-W direction, meters,

EUNSTMX = maximum value of UTM coordinates in the N-S direction, meters,

XDIST = total length of grid in an E-W direction, meters, and

YDIST = total length of grid in a N-S direction, meters.

Starting with the first cell as shown above, all coordinates are cell-centered in both x and y directions. They are used for locating COC sites from UTM coordinates supplied as input as described in Sec. 2.1

4.5 Optional Input and Other Requirements for River/Stream/Wetland Sites

In exposure scenarios that include the consumption of aquatic animals by the animal under study, additional input is required for each grid cell of this type. In this version of ECORSK.5 all cells are considered to be identical and require the following input:

- area, km^2, of each river grid cell,
- area enhancement factor of each river grid cell,
- number of COCs in each river grid cell,
- COC concentration, mg/kg, pCi/g,
- COC background concentration, mg/kg, pCi/g,
- BAF for COC in river/stream/wetland sediment,
- TRV of COC, mg/kg/day, pCi/g, and
- TRV adjustment factor for COC.

The input file *river.dat* contains this information, but data is entered from a terminal, or if this information is not required, then a dummy file is required for proper execution of ECORSK.5. Each cell of this type is then assigned UTM coordinates as follows:

$$CNSTC(n) = EUNSTMN + 30.48\ (YC-1) \quad (12a)$$
$$CEWC(n) = EUEWMN + 30.48\ (XC-1) \quad (12b)$$

where

YC = N-S cell number and
XC = E-W cell number.

Coordinates for other potential release sites (PRSs) are entered as input in the file *eeuinp.dat* as described previously. Also, each river/stream/wetland cell is labeled "river" for identification purposes, whereas other cells are identified by their cell numbers, i.e., 115-100 and are entered as input from the file *eeuinp.dat*. Finally, a sediment ingestion fraction from a given diet of aquatic food such as fish for the bald eagle (Gonzales et al., 1998a) is assigned in these cells in replacement of the soil ingestion fraction. A value of "0" may be assigned to this fraction if it is not used. This procedure, together with pertinent mathematical relationships, is presented in Sec. 1.6. All other types of cells use the fraction of diet as soil. The cells within the river grid are all assigned an identification number of "98" as described in Sec. 2.3.3.

4.6 Nest Site Placement on PRSs or Randomized Placement within a Habitat and Estimation of HRs

The placement of a nest site on a PRS or at random within the nesting habitat of an animal of the EEU is accomplished in several stages. In the selection of a PRS as a nest site within the animal's EEU, the first stage is to locate the x and y coordinates of the PRS on the grid, and then determine whether it is within the EEU. If the value of the cell is equal to "99" as defined in Sec. 2.3.3, then the determination is complete; otherwise the cell is not used for cumulative HQ determination. If the nest site is selected at random from the animal's nesting habitat, then a Monte-Carlo approach is used making sure that the selected nest site is within the animal's nesting habitat (cell value = 99). The grid cell x, y coordinates are determined as follows:

IPX = 1 + [-EUEWMN + CEWC(n)] NX/XDIST (12c)
IPY = 1 + [-EUNSTMN + CNSTC(n)] NY/YDIST , (12d)
where

IPX = cell grid number in the E-W direction,

IPY = cell grid number in the N-S direction,

CEWC(n) = UTM coordinate (E-W) for the *nth* PRS, meters, and

CNSTC(n) = UTM coordinate (N-S) for the *nth* PRS, meters.

The grid cell x, y coordinates of a given random site are determined using Eqs. 12a and 12b above,
where
CNSTC(n) = *INT* (EUNSTMN+YRND*YDIST)(12e)
and
CEWC(n) = *INT* (EUEWMN+XRND*XDIST) (12f)
where
YRND = *ABS*(RANDOM(2)) and (12g)
XRND = *ABS*(RANDOM(2)), (12h)
and

YRND = a random real number between the values (0,1) and

XRND = a random real number between the values (0,1).

A random number seed is entered by the user during input (Sec. 2.2.1) or allows for a seed value of "1000" as a default. Different seed values will result in different random nest site selections and the ordering of such. This routine is ignored if nest sites are being purposely placed on PRSs within the EEU of the animal in question, or if the user selects specific sites for analysis as described earlier. ECORSK.5 ensures that a random site is not picked more than once. The specified number of random nest sites must be less than the total number of grid cells in the nesting habitat.

4.7 Estimating HRs (Grid Cell Selection) Around a Nest Site and Differential Feeding within a HR

The determination of the cumulative number of grid cells within a HR that surround a given nest site within the habitat of an animal can be selected by the user to be one of four types:

1. Selection without regard to HR angle on the EEU and with equal probability of foraging in any surrounding grid cell (square HR or forage site in horizontal direction),
2. Selection with regard to HR angle on the EEU, but with equal probability of foraging in any surrounding grid cell (square forage site at an angle to the horizontal),
3. Selection without regard to HR angle on the EEU, but with unequal probability of foraging in any surrounding grid cell (rectangle in a horizontal direction), and
4. Selection with regard to HR angle and with unequal probability of foraging in any surrounding grid cell (rectangle at an angle from the horizontal).

These options allow the user to orient HRs more realistically within a grid system commensurate with foraging habits of an animal within an EEU and the shape of the HR within it. An iterative routine selects consecutive grid cells for one of the four scenarios outlined above until the sum of the areas exceeds the area of the animal's HR, which has been provided as input or automatically estimated by ECORSK.5 (see Sec. 2.3.1.5). The area of a unit grid cell is estimated as

AREAXY = YDIST XDIST/(NY NX) (13a)

And the HR criteria for a specific animal is satisfied when

$$HR = \sum_{i=1}^{nn} AREAXY_I \qquad (13b)$$

where

$AREAXY_i$ = area of the *ith* grid cell, m^2

and

nn = number of grid cells required to equal the HR.

4.7.1 Horizontal HR and Equal Probability of Foraging

Each specified nest site is first set as a focal point (0,0) for an x, y coordinate system, and cells are systematically selected for the HR through an iterative routine which selects cells with the following x, y coordinates in a given order (Figure 4).

The underlined coordinates in Figure 4 are duplicates of the previous iterations and are ignored when they are encountered more than once by ECORSK.5. The resulting strategy is for ECORSK.5 to select grid cells from the perimeter starting on the lower left (S) and proceeding to the right (W-E); then filling in the perimeter upward (S-N) first on the left side (W), and then on the right side (E). Finally the upper row (N) is selected from left to right (W-E). An ever-enlarging perimeter is filled until Eq. 13b is satisfied. These coordinates are added to the grid cell coordinates (IPX, IPY) estimated from Eqs. 12a and 12b above to obtain the final grid coordinates of the cells included within the HR. The net result is the formation of a square HR around the nest site grid first incrementing the y-axis direction one unit for each x-axis iteration across all units as shown above.

4.7.2 Angled EEU and Equal Probability of Foraging (Square, Angled HR)

A scenario of this type arises when an EEU parallels a canyon wall, stream, or a natural formation at angle to the horizontal (E-W) direction. In this case the tangent of the angle is used (rise / run) to rotate the HR in that direction. Both the x and y coordinates are adjusted as follows:

$$IYI = IYU + IYA , \qquad (14a)$$

where

IYI = grid cell y-coordinate, meters, adjusted for inclination of the EEU from the horizontal (E-W) direction,

IYU = grid cell y-coordinate, meters, unadjusted for inclination, and

IYA = grid cell inclination adjustment, meters

and

$$IYA = (IYU - IYN) SLOPE , \qquad (14b)$$

where

IYN = the y-coordinate of the grid cell containing the nest site, meters, and

SLOPE = fractional slope of the HR from the horizontal on the EEU [INPUT].

The x-coordinate adjusted for rotation is estimated as

$$IXI = (IXU^2 + IYU^2 - IYI^2)^{0.5} , \qquad (14c)$$

where

IXU = grid cell x-coordinate, meters, unadjusted for inclination and

IXI = grid cell x-coordinate, meters, adjusted for inclination of the HR from the horizontal (E-W) direction.

These operations within ECORSK.5 have the effect of tilting the square HR in the desired direction for grid cells with x-coordinates greater or lesser than the x-coordinate of the specific nest site in question.

(0,0)

1st iteration

(-1,-1) (-1,0) (-1,1) (0,-1) (0,0) (0,1) (1,-1) (1,0) (1,1)

2nd iteration

(-2,-2) (-2-1) (-2,0) (-2,1) (-2,2) (-1,-2) (-1,-1) (-1,0) (-1,1) (-1,2) (0,-2) (0,-1) (0,0) (0,1) (0,2)
(1,-2) (1,-1) (1,0) (1,1) (1,2) (2,-2) (2,-1) (2,0) (2,1) (2,2)

3rd iteration

(-3,-3) (-3,-2) (-3,-1) (-3,0) (-3,1) (-3,2) (-3,3) (-2,-3) (-2,-2) (-2,-1) (-2,0) (-2,1) (-2,2)
(-1,-3) (-1,-2) (3,3)

4th iteration

Figure 4. The iterative routine selects cells with x, y coordinates in a given order.

4.7.3 Horizontal HR with Unequal Probability of Foraging

A scenario of this type occurs where the HR does not need to be adjusted for tilt away from the horizontal (E-W) direction, but where its relatively narrow width would justify elongating the HR in parallel with respect to the x-axis. The relationship for this type of transformation is accomplished by adjusting the run (x-axis) greater or lesser than the rise (y-axis) to modify the iteration technique described in Sec. 4.7.1:

$$IXI = IYI\ IAXR - IAXR + 1, \qquad (15)$$

where

IXI = number of iterations in the W-E direction from the nest site,

IYI = number of iterations in the S-N direction from the nest site, and

IAXR = x/y ratio.. 1, 2, 3,...etc.

If the x/y ratio equals 1.0, then IXI equals IYI and a square perimeter is generated around the nest site, otherwise rectangular shapes are generated depending on the value of IAXR as described above.

4.7.4 Angled, Rectangular HR with Unequal Probability of Foraging

A scenario where the EEU is relatively narrow with respect to a HR and where the former is at an oblique angle to the horizontal (E-W) direction may require both HR tilting as described in Sec. 4.7.2, and rectangular HR shaping as described in 4.7.3 above. In such a case, the HR shaping is performed initially assuming a horizontal (E-W) direction before a slope correction of the x- and y-coordinates is applied for proper orientation of the HR around a nest site.

4.7.5 Differential Feeding within a HR

The relationship for differential feeding within the HR was described in Sec. 1.7.3 through the use of the exponential equation presented in Eq. 9e. This equation

is used to modify the intake from a given grid cell with the HR of a given animal on a specific nest site as described earlier. While the application of this option for HI analysis weights cells closer to the nest as contributing most to the simulated foraging process, it does not affect the shape or the angle of the HR. It does affect the enhancement factor which is applied in the execution of Eq. 5 (Sec. 1.3), and works in combination with any or all geometrical modifications of the HR.

4.7.6 Cell Testing for Use in HI Analysis of the HR for Randomly Placed and Assigned Nest Sites

Cell coding was previously described in Sec. 2.3.3 to identify grids (1) outside the EEU (code "0"), (2) inside the EEU, but outside the habitat of a given animal (code "1"), (3) within the nesting habitat (code "99"), and (4) within a lotic or lentic system (flowing or standing water) or wetland (code "98"). In order for a nest site to qualify for HI analysis, it must be located within a nesting habitat for a given animal. In order for cells surrounding a nest site to be included in a HI calculation, they must be located within the EEU, which is comprised of the nesting habitat and the foraging area or HR. This is required because some GIS/ARC/INFO mappings include grid information outside of the EEU that must be excluded from consideration. In addition, ECORSK.5 does not permit any grid cell within the HR to be used in HI calculations more than once by changing the value of a used cell so that it will be excluded from further consideration. Other tests are listed below.

4.8 Tolerance Testing of Cell Locations for PRS and User Selected Sites Within the EEU

All cells including the nest site involved in an HI analysis are tested to be within one cell length in both N-S and E-W directions with respect to a PRS to be included in the calculations for that PRS. That is, any cell which is identified by ECORSK.5 is allowed a tolerance of one cell length in both positive and negative directions N-S and E-W to be included as a PRS cell in the analysis. In this case the nest site has been previously determined to be a PRS or user selected site within the EEU of the animal in question. Having identified a nearby PRS by this method, the next step is to identify the x-, y-cell coordinates of the PRS within the EEU for use in estimating the pHI for that cell to the overall cumulative HI for a given nest site:

$$IXC = 1 + (-EUEWMN + XCRD(J))\ NX/XDIST \quad (16a)$$
$$IYC = 1 + (-EUNSTMN + YCRD(J))\ NY/YDIST\ , \quad (16b)$$

where

IXC = cell coordinates in the E-W direction of the PRS and

IYC = cell coordinates in the N-S direction of the PRS.

All other terms have been defined previously in Sec. 4.4. PRS attributes are then tested for inclusion into Eqs. 6a, 6b, or 8 depending on COC type and behavior. These attributes may include modification of occupancy factors for weighted (or differential) feeding (see Sections 1.7.3 and 4.7.5). All other attributes including COC name and concentrations, TRVs, cell areas, background concentrations of COCs...etc. are entered as input for the given PRS (see Sec. 2.3.2 which describes PRS input file *eeuinp.dat*)

4.8.1 Tolerance Testing of Cell Locations for Randomly Selected Sites within the Habitat

The procedure for tolerance testing of cell locations for randomly selected nest sites within the habitat, and for PRS selections within the EEU are identical to that previously described for PRS nest site within the habitat of the EEU with a few exceptions. The use of Monte Carlo selection of random nest sites was described in Sections 2.2.2, 2.2.7, 2.3.1.1, and 4.6. The random number sequence can be changed if different random selections of nest sites are desired and/or for enveloping estimates of HIs. ECORSK.5 does not allow for any randomly selected site to be duplicated, hence the number of selected nest sites, which is determined by user input, must be commensurate with ($\leq$) the total number of grid cells in the nesting habitat in order to obtain meaningful randomization for different seedings of the random number generator within ECORSK.5. It is not necessary for a nest site to be situated on a PRS within the nesting habitat to qualify a nest site for HI analysis using the randomization strategy.

5.0 Description of Output from ECORSK.5

Output from ECORSK.5 is either cumulative or statistical in nature. Cumulative output may reflect partial or total information, while statistical output assumes that the variables being tested are normally distributed in the determination of mean and standard errors. Non-parametric statistics may apply when distributions depart from normality. These and other aspects concerning data reduction are presented in the following sections.

5.1 Cumulative Output from ECORSK.5

The output in its rawest (most broken down) form from ECORSK.5 is a pHQ for each COC within each grid cell of an HR for a given nest site. This is reported for the specified number of nest sites, which for the examples previously cited was 100. The raw output can get quite lengthy. This is embodied in Eqs. 6a and 6b (Sec. 1.4) or Eq. 8 (Sec. 1.5). This output is considered "source" data because it is a contributor to the HI of any given nest site. In addition, these equations embody information for a given nest site whereby pHQs for all COCs and all grid cells within a HR are summed in a cumulative fashion:

$$HI_m = \sum_{i=1}^{n} \sum_{j=1}^{coc} pHQ_{m,i,j}, \qquad (17a)$$

where

HI_m = the cumulative HI for the *mth* nest site,

$pHQ_{m,i,j}$ = the partial hazard quotient contributed to the *mth* nest site by the *ith* PRS on the *jth* COC,

n = number of cells in the HR of the animal surrounding the *mth* nest site, and

coc = the number of COCs in the *ith* grid cell.

Thus, hq.dat contains an HI for each of the number of nest sites specified by the user. The arithmetic mean of these HIs is reported in the output file *outrsk.dat*. The arithmetic mean of the HIs and the HI for each nest site represent the highest levels of "roll-up" (or summary) data. Output for Eq. 17a is located in the file *hq.dat*.

The number of grid cells (n) contributing to the HI for a given animal depends on its body mass (see Sec. 2.3.1.5, Eqs. 10a-10e), while the number of COCs depends on the specific PRS in question. In

many instances a grid cell within the HR will not contain any COCs, but is taken into account when estimating mean values of this statistic over all nest sites (Eq.17a is set to zero). Cumulative HQs of different types (or "roll-ups") are also estimated for all COCs for each grid cell located within the HR of all nest sites:

$$pHQ_{m.k} = \sum_{j=1}^{coc} pHQ_{m.k.j}\,, \qquad (17b)$$

where

$pHQ_{m.k}$ = the partial HI from the *kth* grid cell in the HR of the *mth* nest site for all COCs,

$pHQ_{m.k.j}$ = the partial HI from the *kth* grid cell in the HR for the *mth* nest site for the *jth* COC,

The output for Eq. 17b is located in the file *hqp.dat*. The cumulative values in these files are utilized to obtain statistical parameters described in the next section. An example of *hqp.dat* output was shown in Table 4. An example of *hq.dat* is provided in Table 5.

A partial cumulative HQ can also be obtained for each COC for a given nest site using the following relationship:

$$pHQ_{m.j} = \sum_{k=1}^{p} pHQ_{m.k.j}, \qquad (17c)$$

where

$pHQ_{m.j}$ = the partial HI for the *mth* nest site from the *jth* COC for all contaminated grid cells,

$pHQ_{m.k.j}$ = the partial HI for the *mth* nest site from the *jth* COC and the *kth* grid cell, and

n = the number of cells in the HR of the animal surrounding the *mth* nest site.

A listing of these partial cumulatives are stored in the file *hqpc.dat* as ECORSK.5 output. An example of *hqpc.dat* output was shown in Table 4.

5.2 Statistical Output from ECORSK.5

The estimation of HIs from a number of nest sites of a random or selected nature and the need to express these results in a single inferential formulation reflective of all nest sites makes it necessary to express the results in mean and standard error formulation. The formulation may take the form of parametric or non-parametric tests depending on the divergence from normality of the HI distribution from all nest sites involved. Small or insignificant departures of this type generally yield the same results by either method (Gallegos et al. 1997a), hence, the parametric form is programmed in ECORSK.5 based on the assumption that the investigator will test for any significant departures from the normal distribution and/or use the appropriate parametric or non-parametric method if necessary. In all cases encountered through the use of either method, the results have been nearly equivalent (Gallegos et al., 1997a).

5.2.1 Mean and Standard Deviation of HIs from all Nest Sites

The mean HI over all nest sites for a given scenario is simply an extension of Eq. 17a:

$$MHI = \sum_{m=1}^{n} HI_m/n\,, \qquad (18a)$$

where

MHI = The mean HI for a given habitat from all nest sites.

Table 5. Examples of Partial Output File of *hq.dat* Generated by ECORSK.5 for an Assessment of the Southwestern Willow Flycatcher (Source: Gonzales et al., 1998b).

Columns 1 and 2 = nest x, y coordinate; 3 = HI for a given nest (cumulative HQ of all grid cells for all COCs in an HR); Column 4 = Nest site no. or index.			
69	62	2.30404	40
44	118	0.000000E+00	41
85	34	0.000000E+00	42
79	50	0.000000E+00	43
81	47	0.000000E+00	44
44	119	0.000000E+00	45
85	39	0.000000E+00	46
44	120	0.000000E+00	47
63	69	0.246128	48
56	85	0.000000E+00	49
84	43	0.000000E+00	50

The standard error is estimated from the statistic HI_m for each nest site using the conventional method for a normal distribution. All cells in the HR are included for analysis including non-contaminated ("background") grid cells. Output of this type for all nest sites is included in the output file *outrsk.dat*. An example of *outrsk.dat* is provided in Table 6.

5.2.1.1 Mean Partial HI of each Nest Site for all COCs and all Contaminated Grid Cells

The mean partial HI from all PRSs and COCs located within the HRs of all nest sites is estimated with the following relationship which is an extension of Eq. 17b.

$$MPR = \sum_{k=1}^{np} pHQ_k/np \qquad (18b)$$

where

MPR = the arithmetic mean HI of all nest sites (cumulative for all COCs).

Only those cells which are identified as contaminated within the HR of a given nest site are utilized in making this estimate, hence it is useful in identifying grid cells that are major contributors to the overall HI for a given nest site and for comparison to the mean value. The standard error is estimated from the statistic $pHQ_{m,k,j}$ using the conventional method for a normal distribution. Output of this type for all nest sites and PRSs is included in the output file *outrsk.dat*.

5.2.1.2 Mean Partial HI from all COCs in all PRSs for all Nest Sites

The mean partial HI for all PRSs and COCs located in all nest sites used in an HI analysis is an extension of Eq. 17a, but with the nest site included in the summation:

$$HIU = \sum_{m=1}^{ns} \sum_{i=1}^{np} \sum_{j=1}^{coc} pHQ_{m,i,j}/(ns\ np\ coc);\quad pHQ_{m,i,j} > 0.0, \qquad (18c)$$

where

HIU = mean total HI for all partial HI calculations in the analysis where the latter is greater than zero and

Table 6. Partial File of *outrsk.dat* for an Assessment of the Southwestern Willow Flycatcher (Source: Gonzales et al. 1998b).

you have selected coc specification = 1.00000
you have selected specific run option = 3.00000

you have selected exponential feeding option = 0.000000E+00
the home-range slope frac. around a nest site = 0.000000E+00
you have selected X/Y ratio around nest site = 1.00000

ECOLOGICAL RISK INPUT SUMMARY
using ECORSK, Version 1

program run on 04/09/98 by gjg, test of flycat3.exe (ecorsk5.exe)
you have selected random seed number = 1000
ANIMAL = willow flycatcher

ANIMAL TYPE SELECTED FOR willow flycatcher IS SPECIFIED AS 2
1 = MAMMAL, 2 = BIRD, 3 = REPTILE, AND 4 = AMPHIBIAN
FEEDING TYPE FOR willow flycatcher IS SELECTED AS 10.0000,
10 = CARNIVORE,100 = HERBIVORE, AND 1000 = AMPHIBIAN

BODY WEIGHT,KGFWT,FOR willow flycatcher = 1.500000E-02
soil intake, fraction of food ingestion, for willow flycatcher = 5.000000E-02
EFFECTIVE SED. INTAKE FRAC. FOR willow flycatcher = 0.000000E+00
THE AREA, KM2, OF THE EEU FOR willow flycatcher IS 10.2180

THE MAX. AND MIN. N-S UTM COORD. FOR willow flycatcher ARE 1.763338E+06 1.751438E+06
THE MAX. AND MIN. E-W UTM COORD. FOR willow flycatcher ARE1.651572E+06 1.634172E+06

END OF ECOLOGICAL RISK INPUT SUMMARY

ECOLOGICAL RISK OUTPUT SUMMARY
using ECORSK, Version 1

THE AREA,KM^2, OF THE HOME-RANGE FOR willow flycatcher IS 2.632225E-02
FOOD CONSUMPTION,KGFWT/DAY, FOR willow flycatcher IS 3.780579E-03

for willow flycatcher maximum E-W distance of EEU in FEET = 17400.0
For willow flycatcher maximum N-S distance of EEU in FEET = 11900.0

mean total HQ for willow flycatcher, all RANDOM sites; col.1 = mean, col. 2 = mean std. err, col. 3 = df
0.120118 0.445413 100.000

mean partial HQ for willow flycatcher RANDOM X PRS; col.1 = mean, col. 2 = mean std. err, col. 3 = df
0.261126 1.777112E-02 46.0000

mean partial HQ for willow flycatcher RANDM X PRS X PRS X COC
col.1 = mean, col. 2 = mean stnd. error, col. 3=DF
5.830966E-03 1.954585E-02 2060.00

MEAN HQ FOR willow flycatcher BY COC;
COL.1=MEAN, COL.2 = MEAN STND. ERROR, COL.3=OBS

4.699031E-05	7.421651E-06	46.0000	Trinitrotoluene [2,4]	1
1.097407E-04	2.828602E-05	46.0000	Dinitrotoluene [2,4-]	2
2.823285E-04	1.047368E-04	46.0000	RDX	3
0.000000E+00	0.000000E+00	46.0000	Amino-2,6-dinitrotoluene	4
3.440155E-06	1.733203E-06	46.0000	HMX	5
0.000000E+00	0.000000E+00	46.0000	Amino-4,6-dinitrotoluene	6

ns = number of nest sites used in the HI analysis.

The summation of all partials which meet the above condition is usually less than the denominator shown above (ns np coc), and is calculated by ECORSK.5 each time this condition is met for the entire set of partials estimated under these conditions. The condition requiring finite values for individual estimates of pHIs allows one to compare this value with that obtained in all previous mean estimates. The standard error is estimated from the statistic ($pHQ_{m,i,j}$) using the conventional method for a normal distribution. Output of this type for all nest sites, PRSs, and COCs are included in the output file *outrsk.dat.*

5.2.2 The Mean Partial HI for all Nest Sites for a Specific COC

The mean partial HI for all nest sites for a specific COC is an extension of Eq. 17c described in Sec. 5.1 above:

$$MpHQ_j = \sum_{k=1}^{nsp} \sum_{m=1}^{np} pHQ_{k,m,j}/nsp,\ pHQ_{k,m,j} > 0.0, \quad (18d)$$

where

$MpHQ_j$ = mean partial HI across all nest sites for the *jth* COC, and

nsp = number of nest sites where the *jth* COC is present.

The standard error is estimated from the statistic ($pHQ_{k,m,j}$) using the conventional method for a normal distribution. Output of this type for all nest sites and COCs is included in the output file *outrsk.dat.*

6.0 EEU Grid Data for Three-dimensional Presentation

Cell coded information on the z-axis of the x-, y-coordinate system of the EEU is generated by ECORSK.5 and stored in the file *habit.dat.* The x, y coordinates are given in integer form...(2, 3), (34, 20)...etc. and are a transformation of the original UTM coordinate supplied as input. The z-coordinate is used to identify the type of cell under consideration:

- Cells outside the EEU grid boundary are given the value "0".
- Cells located within the EEU but outside the HR for the specific nest under consideration are given the value "1".
- Cells located within the HR of a specific animal are given the value "4".
- Cells located within the nesting habitat area are given the value "6".
- The cell which identifies the specific nest under consideration is given the value "10".

A modulus selection is requested by ECORSK.5 to store detailed results for the specified number of nests in the file. For instance if the value "50" is entered for this parameter, then ECORSK.5 will store detailed information for the 50th, 100th, 150th nest site...etc. in *habit.dat* for inspection or for graphics presentation. Since the amount of storage required for just one nest can be quite large, the user should be careful with regard to modulus assignment to keep file storage memory requirements to a reasonable level.

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