CHARACTERIZING AQUATIC ECOLOGICAL RISKS FROM PESTICIDES USING A DIQUAT DIBROMIDE CASE STUDY III. ECOLOGICAL PROCESS MODELS

STEVEN M. BARTELL,*† KYM ROUSE CAMPBELL,† CYNTHIA M. LOVELOCK,†‡ SHYAM K. NAIR,† and JENNIFER L. SHAW§
†The Cadmus Group, 136 Mitchell Road, Oak Ridge, Tennessee 37830, USA
‡Institute for Environmental Modeling and Department of Mathematics, University of Tennessee, Knoxville, Tennessee 37996, USA
§Zeneca Ag Products, DCC II, 1800 Concord Pike, Wilmington, Delaware 19850-5458, USA

(Received 15 January 1999; Accepted 8 September 1999)

Abstract—The purpose of this study was to extend the set of risk characterization approaches developed in an earlier study beyond simple comparisons of exposure and effects (e.g., quotients, overlapping frequency distributions) through use of ecological models. These models were used to evaluate the ecological risks from diquat dibromide for individual Daphnia using an individual-oriented model, a population of bluegill sunfish (Lepomis macrochirus) using a demographic model, and ecological communities within a generic lake in Central Florida, USA, using the Comprehensive Aquatic Systems Model. The ecological models presented in this study more realistically address the potential risks posed by pesticides to individual organisms, populations, communities, and ecosystems than risk assessment methods based on simple comparisons of exposure and effects. The ecological impacts calculated by these models support the inference of minimal risks being posed by diquat dibromide to aquatic systems as concluded from previous empirical comparisons of exposure and toxicity data.

Keywords—Ecological risk assessment Diquat dibromide Individual-oriented model Demographic model Eco-

INTRODUCTION

In a previous study [1], a set of strictly empirical methods for estimating ecological risk was presented using exposure estimates and toxicity data quantifying the environmental fate and ecological effects of diquat dibromide in regional lake and pond scenarios. These methods ranged from single-value quotient calculations to comparisons of distributions of exposure to distributions of toxicity data using Monte Carlo simulations. One advantage of these calculations lies in their computational simplicity. Also, the results are easily interpreted for increasingly high or vanishingly small quotient values. However, the quotients become less useful in decision making as their values exceed, or that fail to exceed, the decision value. Perhaps the greatest limitation in these strictly empirical approaches is the absence of process-level (i.e., causal, mechanistic) relationships between exposure and expected ecological impacts of pesticides.

The purpose of this study was to extend the risk assessment beyond simple, purely empirical approaches by using different kinds of ecological models. The modification and implementation of ecological models present one potentially powerful method for characterizing the ecological risks posed by pesticides. Importantly, each modeling approach attempts to represent mathematically the physical, chemical, biological, and ecological processes that mechanistically translate exposure into one or more adverse ecological effects; these models integrate exposure and effects to estimate risk. These mechanisms are, at best, implicit in the sequence of hazard quotients as calculated previously [1]. The increasing reliance on ecological models for the risk assessment of pesticides underscores the need to develop further such modeling capabilities. In this study, ecological models were used to evaluate the risks posed to individual organisms, populations, communities, and ecosystems from exposure to diquat dibromide in representative aquatic environments selected from the previous study [1].

The ecological models used in this study are described and used to assess the ecological risks posed by diquat dibromide herbicide. The strictly empirical methods presented earlier [1] consistently suggested that diquat dibromide posed negligible ecological impacts to nontarget aquatic organisms for realistic application scenarios in different geographical regions. The working hypothesis of this study is that ecological models will similarly suggest a minimal ecological risk posed by diquat dibromide for the same exposure profiles as used previously [1]. This study also addresses the strengths and limitations of these ecological modeling approaches for risk assessment. Together, the set of methods presented in the first study [1] and the ecological models described here are offered as one possible comprehensive methodology for effectively assessing the ecological risks posed by pesticides and other toxic chemicals. The ecological modeling approaches examined in this study appear to be consistent with the aims and goals expressed by the Aquatic Risk Assessment and Mitigation Dialogue Group [2].

ECOLOGICAL MODELS FOR RISK CHARACTERIZATION

The different types of ecological models used in this study are described here. Each modeling approach merely reflects one particular view of the same ecological systems. The models are not offered as a progression from simple to complex...
ecological models but as a set of modeling tools for estimating ecological impacts and characterizing ecological risks. Similarly, this demonstration is not intended to recommend or identify a best ecological modeling approach for assessing the risks posed by pesticides. Such recommendations based on this (or any other) modeling study would be merely speculative.

**Daphnia sp. individual-oriented model**

Individual-oriented models (IOMs) can be used to assess the risks posed by pesticides on individual organisms. One advantage of an IOM is that disparately scaled phenomena, including life-history traits, behavior, growth, reproduction, and other biological or ecological characteristics, for an individual organism can be formulated using a common mathematical and mechanistic framework [3]. IOMs have been developed for wading birds [4] and panthers (D.L. DeAngelis, personal communication) and several species of fish [5,6]. Available IOMs might be modified to simulate the direct uptake of dissolved pesticides across gill membranes similar to the approach used in the Food and Gill Exchange of Toxic Substances model for fish [7]. In addition, IOMs have been developed to examine the accumulation of nonpolar organic contaminants by zooplankton [8,9].

In this study, the model developed by Hallam et al. [8] was adapted to assess the effects of diquat dibromide on the various life stages of *Daphnia*. The Hallam et al. model is based on the energetics of an individual female *Daphnia* following its life history from egg to juvenile to adult instar. Each organism consists of two modeled components, lipid and structure (protein and carbohydrates), with each component consisting of a labile and a nonlabile portion. The dynamics of an individual *Daphnia* are represented by two coupled, ordinary differential equations that describe the rates of change for the mass of the lipid and the mass of the structure in *Daphnia*. These rates are determined by the difference in the inputs, as represented by the growth of the lipid and the structure compartments, and in the outputs, as manifested by losses from the lipid and the structure compartments. Lipid and structure of an individual *Daphnia* increase from feeding on a resource that also has lipid and structure components. The amount of food resource converted to viable energy is based on the assimilation efficiencies of the lipid and the structure. The losses consist of lipid and structure allocation for egg production and energy allocation for maintenance, work (activity), and reproduction (Fig. 1). The model of individual growth was incorporated into a system of McKendrick-von Foerster partial differential equations to describe the growth dynamics of a population of individual *Daphnia* [8].

The physiological energetics–based model of individual *Daphnia* [8] coupled with an exposure model, the Food and Gill Exchange of Toxic Substances model [7], was used to assess the effects of diquat dibromide herbicide on the age structure of a model *Daphnia* population. The individual model, which was used previously to study the mortality effects of chemicals on populations [9] and the effects of sublethal narcosis on growth [10], was modified to reflect the chemistry and toxicology of diquat dibromide. The octanol-water partition coefficient, $K_{ow}$, used to estimate exposure to diquat dibromide herbicide was $10^{4.4}$ at 20°C [11]. The toxicity values used in the model for the no-observed-effects concentration, the 50th-percentile effects concentration (EC50) for growth, and the 50th-percentile lethal concentration (LC50) specific to *Daphnia magna* for diquat dibromide herbicide were 0.0465 [12], 1.6 [13], and 3.0 mg/L [13], respectively.

Each *Daphnia* simulation described a 50-d, chronic exposure to diquat cation at two time-weighted mean concentrations, 0.048 and 0.0263 mg diquat cation/L. The exposure concentration of 0.048 mg diquat cation/L was the highest 90th-percentile exposure value simulated by the Exposure Analysis Modeling System (EXAMSII) lake scenario for all regions of the United States for the 48-h duration, and 0.0263 mg diquat cation/L was the highest 48-h exposure value simulated for the EXAMSII farm pond scenario for all United States regions [14]. A *Daphnia* IOM simulation using zero exposure provided a baseline reference for risk estimation.

**Bluegill sunfish demographic model**

Demographic (or Leslie matrix) models have been well-developed in quantitative ecology [15–17]. Demographic models have also been used in ecological risk assessments for populations of fish [18–23]. In this study, a demographic model developed for the bluegill sunfish (*Lepomis macrochirus*) [23] was modified to estimate the effects of diquat dibromide on the abundance of different life stages and total population size of bluegill (Fig. 2). The overall approach required modification of a population model for bluegill sunfish, development of a diquat dibromide toxicity data set for selected life stages of bluegill, and derivation of exposure-response functions that equated diquat dibromide toxicity with changes in the basic parameters of the model.

A demographic model typically describes a population as a set of discrete age or size classes, each containing a specified initial number of individuals [17]. At successive time intervals,
members survive to the next age class with a probability $S_i$. Reproductive individuals in each stage also contribute some number of progeny, $F_i$, to the first age class during this same time interval. The number of individuals in each stage $i$ at any time $t$, as represented by $n_i(t)$, is determined by the number that mature and survive from the previous stage (controlled by $S_i$), the number that advance to the next stage (controlled by $S_{i-1}$), and the number that die within the stage (controlled by both $S_i$ and $S_{i+1}$). The survivorship and fecundity parameters for each class are summarized in a production or Leslie matrix [24]. Projections of future population size and structure are made using the Leslie matrix and a vector of the initial conditions.

Functional relationships between fish exposure to pesticide and values of the survivorship and fecundity parameters were derived for use in the demographic model to assess the risks posed by pesticides. Bartell and Wittrup [25] used a function developed by Barnthouse et al. [19] that equates exposures to toxic metals with changes in demographic parameters for a population of northern pike (Esox lucius). This exposure-response function was developed using data for 77 different chemicals, including pesticides.

The model is presented in matrix form as

$$
\begin{align*}
\begin{bmatrix}
    n_1^{(N+1)} \\
    n_2 \\
    n_3 \\
    \vdots \\
    n_m \\
\end{bmatrix} &=
\begin{bmatrix}
    F_1 & F_2 & F_3 & \ldots & F_m \\
    S_2 & 0 & 0 & \ldots & 0 \\
    0 & S_3 & 0 & \ldots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & S_4 & \ldots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & \ldots & S_m \\
\end{bmatrix}^{\top}
\begin{bmatrix}
    n_1^{(N+1)} \\
    n_2 \\
    n_3 \\
    \vdots \\
    n_m \\
\end{bmatrix} \\
\end{align*}
$$

(1)

where $n_i(t)$ is the number of individuals in size-stage $i$ at time $t$, $n_i(t + 1)$ is the number of individuals in size-stage $i$ at time $(t + 1)$, $S_i$ is the fraction of $n_i(t)$ surviving to stage $i$ during the time interval, $F_i$ is the reproductive contribution of each stage $i$ to stage 1, and $m$ is the total number of stages. In matrix notation, Equation 1 can be represented as $N(t + 1) = L \times N(t)$, where $L$ is the Leslie matrix. The time or projection interval in the model is typically the same as the stage interval. The initial population distribution within various stages is usually obtained from field data [23].

One limitation of Leslie matrix models is that unless the survivorship and reproduction parameters in Equation 1 are perfectly balanced, the population numbers necessarily increase without bound, decrease to zero, or oscillate through time [17]. In addition, when the time interval of interest is less than the stage interval, Equation 1 does not adequately represent the dynamics of population change. This temporal scaling becomes important when assessing risks posed by the typically short-term, pulsed exposures involved in the application of diquat dibromide and other pesticides.

Equation 1 also does not address the ratio of females to males in the mature stages of the population and, therefore, does not truly represent the number of eggs and larvae added to stage 1. To address these shortcomings, the bluegill demographic model was reformulated as Equation 2 (Fig. 2):

$$(n_{10})^{(N+1)} = \begin{bmatrix}
    S_{11} & r_2F_2 & r_3F_3 & \ldots & r_mF_m \\
    S_{12} & 0 & 0 & \ldots & 0 \\
    0 & S_{22} & S_{23} & \ldots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & S_{34} & \ldots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & \ldots & S_{m-1} \\
\end{bmatrix}
\begin{bmatrix}
    n_{11}^{(N+1)} \\
    n_2 \\
    n_3 \\
    \vdots \\
    n_m \\
\end{bmatrix}

(2)

where

$$
n_1 = \alpha n_{10} \exp(-\beta n_{10}),
$$

(3)

$$
F_i \neq 0 \quad \text{during the spawning season},
$$

(4)

$$
S_{i-1} = 0 \quad \text{after the spawning season},
$$

(5)

$$
n_{1a} = n_{11} \quad \text{after the spawning season},
$$

(6)

In Equation 2, $t$ represents a daily time step used to model the growth of the population, and $n_{10}$ represents the population of eggs and larvae produced by the mature female populations in stages 2 through $m$. The simulations are assumed to begin on the day of first spawning (i.e., $t = 1$ on the first day of spawning). The population $n_{1a}$ in stage 1 of Equation 2 is a function of time as presented in Equation 6. During the spawning season, the growth of individuals from stage 1 to stage 2 occurs each day based on the population in stage 1 at the beginning of the spawning season as a function of $S_{11}$ (Fig. 2). In Equation 6, $n_{11}$ represents the population in stage 1 ($n_i$) at $t = 1$, the first day of spawning. In Equation 2, $S_{11} = 1$ represents the fraction of the population in stage $i$ that grows to stage $i$. The population in each stage $i$ ($i > 1$) during the spawning season is based on the growth of the population from the previous stage (controlled by $S_{i-1}$) and the survivorship of the population within the stage (controlled by $S_i$). For stage 1, during the spawning season, the growth of the population is controlled by the production of eggs and larvae from the populations in all other stages ($n_i$ through $n_{10}$) and controlled by $r_2F_2$ through $r_mF_m$, the survivorship and growth of eggs and larvae to stage 1 fish (controlled by Eqn. 3), and the survivorship of the stage 1 population (controlled by $S_{11}$). Here, $r_i$ represents the fraction of the female population in stage $i$, and $F_i$ represents the fecundity of stage $i$ expressed as the number of eggs and larvae produced per female in stage $i$. It should be noted that fish in stage 1 before the spawning season do not survive through the spawning season, because they either grow into stage 2 fish or die. Therefore, as $n_{11}$ takes on a value of $n_{1a}$ during the spawning season, $S_{11}$ takes a fixed value in such a manner that no fish in stage 1 at the end of the spawning season were in stage 1 during the previous year. Therefore, at any time during the spawning season, the population of fish in stage 1 represents newly born fish and the previous year’s fish that have survived, as represented by $n_1$ in Equation 3.

In this revised demographic model, the production of eggs
and larvae occurs only during the spawning season, by definition. After the spawning season, $F_1$ becomes zero (Eqn. 4). Therefore, the succession from one stage to the next will only occur during the next spawning season if the stage interval is considered to be one year, as reflected in Equation 5, where $S_{i-1}$ takes on nonzero values only during the spawning season. $S_i$ represents the survivorship of the population within stage $i$; in other words, any reduction in the population within stage $i$ because of death is accounted for as $(1 - S_i)$. That is, the growth of the population in stage $i$ ($i > 1$) after the spawning season is controlled only by the survivorship $S_i$.

Table 1 provides the information [23] used to develop values of the input parameters for Equations 2 through 6. In Equation 3, $\alpha$ and $\beta$ are empirical regression constants that provide density-dependent relationships between the number of eggs and larvae produced during the spawning season and the stage 1 population [23]. Ferson [23] conducted the simulation using the Leslie matrix presented in Equation 1 for an annual time step and with the Ricker's model for density dependence. Ferson's results were reproduced using 400 Monte Carlo simulations [23]. A single reference simulation was also performed using Equation 1 and best-estimate values from Table 1 during the spawning period.

Using this demographic modeling approach, the impacts of exposure to diquat dibromide were expressed as decreases in the fecundity, survivorship, and growth parameters ($F_i$, $S_i$, and $S_{i-1}$, respectively). Separate probit functions were used to describe these exposure-response relationships for diquat using existing toxicity data for bluegill sunfish. The 96-h LC50 diquat dibromide toxicity data for the bluegill [1] resulted in a mean LC50 value of 29.2 mg diquat cation/L (standard deviation, 6.4). The 95% confidence interval of the mean LC50 value was estimated as ±20.8 mg diquat cation/L. Separate probit functions were defined by repeated, random selections of values ($n = 400$) from a uniform distribution of 96-h LC50 values (minimum, 8.3 mg diquat cation/L; maximum, 50 mg diquat cation/L). Development of these functions also assumed that the probit-versus-exposure curve was a straight line passing through the LC50 and the origin. The highest 90th-percentile estimate of the 96-h, time-weighted mean exposure concentration resulting from the EXAMSII lake scenario (i.e., segment B) simulations (0.0263 mg diquat cation/L) for all regions of the United States was used to develop a time series of daily exposure concentrations in combination with the 400 exposure-response functions to estimate the potentially harmful effect on the bluegill population [14]. The 96-h weighted average was used to define daily exposures, because the exposure-response functions were developed from 96-h LC50 values.

### Comprehensive Aquatic Systems Model

The Comprehensive Aquatic Systems Model (CASM) was used to assess the risks posed by diquat dibromide at the scale of aquatic communities and ecosystems (Fig. 3). The CASM is a flexible modeling framework that permits specification of
multiple populations (taxonomically and functionally) of aquatic plants and animals [26]. This flexibility in ecological structure permits definition of generic or site-specific food webs depending on the focus of the assessment and the availability of data. The version of the CASM used here to evaluate pesticides was modified from a previous model developed to examine relationships between food web structure, nutrient cycling, and stability [26].

**Primary producer populations.** Primary producer populations in the CASM can include from one to 10 populations each of phytoplankton, periphyton, and rooted aquatic plants (i.e., macrophytes). Representative species can be selected based on generic regional aquatic ecosystems. Ten species of phytoplankton, five species of periphyton, and five species of macrophytes were selected as being representative of lakes in Central Florida, USA (Table 3).

**Consumer populations.** Consumer populations can include as many as five populations each for eight trophic or functional guilds of grazers and predators, including zooplankton, pelagic omnivorous fish, pelagic piscivorous fish, benthic insects, other benthic invertebrates, benthic omnivorous fish, benthic piscivorous fish, and decomposers. Five species of zooplankton, five species of pelagic omnivorous fish, three species of pelagic piscivorous fish, five species of benthic invertebrates, five species of benthic omnivorous fish, and one species of benthic piscivorous fish were selected as being representative of lakes in Central Florida, USA (Table 3).

**Water quality.** Water-quality characteristics modeled in the CASM include the concentrations of dissolved inorganic nitrogen, phosphorus, dissolved silica, dissolved oxygen, dissolved organic matter, particulate organic matter, and water temperature. The CASM simulates daily values of these state variables based on an overall mass-balance approach that includes external inputs to the aquatic ecosystem, internal uptake, and recycling of nutrients.

**Spatial and temporal scales.** The CASM simulates the daily production dynamics of each state variable for the period of one year. Production dynamics are computed as grams of carbon (gC) and integrated over the water column as defined by the depth of the system. The resulting biomass is expressed as gC/m²; process rates are expressed as gC/m²/d, gC/gC/d, or 1/d depending on the process modeled. State variables that define water quality are output in volumetric units (e.g., µgP/m³, mg dissolved oxygen/L).

The CASM simplistically represents a thermally stratified lake or reservoir as a two-box system with a static epilimnion overlying a constant-depth hypolimnion. The onset of thermal stratification as well as the mixing of these layers are determined by user-supplied values of daily water temperatures in site-specific assessments.

**Bioenergetics equations for producers.** Biomass values of the modeled populations as well as the values of the water-quality state variables are calculated in the CASM by a set of coupled, first-order, linear-differential equations with several nonlinear terms. These equations were derived to describe in aggregated form the more detailed physiological processes that determine growth. The CASM equations are based on energetics (i.e., joules) of anabolic and catabolic processes, but they are computed as units of carbon.

The daily value of biomass (gC/m²) for each modeled population ($B_i$) of phytoplankton, periphyton, and macrophytes is determined by the following equation [27–29]:

$$dB_i/dt = \text{photosynthesis} - \text{respiration} - \text{sinking}$$

or

$$\frac{dB_i}{B_{idt}} = Pm_i \cdot \left( h(T) \left( \beta \exp \left( I_{i}/I_{s_i} \cdot \exp \left( -0.1 \sum_i B_i - 2.0 \right) \right) - \exp(-I_{i}/I_{s_i}) \right) \right)$$

$$\times \min \left( \frac{N}{kN_{i}}, N^{1/P}+P, \frac{S}{kS_{i}}+S \right) - r_i \cdot h(T)$$

$$- \left( s_i + m_i \right) - \sum j h(T) \cdot B_j \cdot C_{ij} \cdot w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_i$$

$$+ \left( B_j + \sum w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_i \right)$$

where

- $B_i$ = the biomass of population $i$ (gC/m²),
- $Pm_i$ = the maximum rate of growth (1/d),
- $h(T)$ = the temperature dependence of growth (unitless),
- $I_s$ = the incident surface light intensity (Eins photosynthetically active radiation/m²/d),
- $I_e$ = the light-saturation coefficient for population $i$ (Eins photosynthetically active radiation/m²/d),
- $N$ = the concentration of dissolved inorganic N (g/L),
- $P$ = the concentration of dissolved inorganic P (g/L),
- $Si$ = the concentration of dissolved inorganic Si (g/L),
- $kN_i$ = the half-saturation constant of N for population $i$ (g/L),
- $kP_i$ = the half-saturation constant of P for population $i$ (g/L),
- $kS_i$ = the half-saturation constant of Si for population $i$ (g/L),
- $r_i$ = the respiration rate for population $i$ (1/d),
Table 3. Comprehensive Aquatic System Model initial biomass values and bioenergetics growth parameters (units) used in Central Florida, USA, lake risk assessment for diquat dibromide

<table>
<thead>
<tr>
<th>Phytoplankton</th>
<th>0.06E+00</th>
<th>18</th>
<th>98</th>
<th>2.00</th>
<th>0.010</th>
<th>14</th>
<th>65</th>
<th>0</th>
<th>0.005</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ankistrodesmus sp.</td>
<td>0.06E+00</td>
<td>18</td>
<td>130</td>
<td>1.80</td>
<td>0.010</td>
<td>12</td>
<td>75</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Kirchneriella sp.</td>
<td>0.10E+00</td>
<td>14</td>
<td>114</td>
<td>1.50</td>
<td>0.010</td>
<td>10</td>
<td>70</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Cryptomonas sp.</td>
<td>0.20E+00</td>
<td>16</td>
<td>110</td>
<td>2.00</td>
<td>0.010</td>
<td>10</td>
<td>75</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Dinobryon sp.</td>
<td>0.50E+00</td>
<td>10</td>
<td>120</td>
<td>1.25</td>
<td>0.020</td>
<td>20</td>
<td>85</td>
<td>1500</td>
<td>0.005</td>
</tr>
<tr>
<td>Diatom sp.</td>
<td>0.20E+00</td>
<td>10</td>
<td>110</td>
<td>1.25</td>
<td>0.020</td>
<td>20</td>
<td>87</td>
<td>1500</td>
<td>0.005</td>
</tr>
<tr>
<td>Fragillaria sp.</td>
<td>0.10E+00</td>
<td>10</td>
<td>125</td>
<td>1.25</td>
<td>0.020</td>
<td>20</td>
<td>90</td>
<td>1500</td>
<td>0.005</td>
</tr>
<tr>
<td>Melosira sp.</td>
<td>0.10E+00</td>
<td>10</td>
<td>100</td>
<td>2.20</td>
<td>0.050</td>
<td>18</td>
<td>70</td>
<td>750</td>
<td>0.005</td>
</tr>
<tr>
<td>Rhodoma sp.</td>
<td>0.05E+00</td>
<td>16</td>
<td>122</td>
<td>1.50</td>
<td>0.010</td>
<td>18</td>
<td>85</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Cyanophytes sp.</td>
<td>0.01E+00</td>
<td>20</td>
<td>112</td>
<td>1.50</td>
<td>0.010</td>
<td>18</td>
<td>70</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Periphyton</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flagellates</td>
<td>0.20E+00</td>
<td>12</td>
<td>112</td>
<td>1.80</td>
<td>0</td>
<td>18</td>
<td>50</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Chrysophytes sp.</td>
<td>0.10E+00</td>
<td>14</td>
<td>100</td>
<td>1.20</td>
<td>0</td>
<td>10</td>
<td>50</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Chlorophytes sp.</td>
<td>0.20E+00</td>
<td>10</td>
<td>115</td>
<td>1.50</td>
<td>0</td>
<td>18</td>
<td>60</td>
<td>750</td>
<td>0.005</td>
</tr>
<tr>
<td>Cyanophytes sp.</td>
<td>0.10E+00</td>
<td>16</td>
<td>125</td>
<td>1.30</td>
<td>0</td>
<td>12</td>
<td>70</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Macrophytes</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Myriophyllum sp.</td>
<td>0.20E+00</td>
<td>22</td>
<td>112</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Elodea sp.</td>
<td>0.20E+01</td>
<td>20</td>
<td>130</td>
<td>0.05</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Ceratophyllum sp.</td>
<td>0.50E+01</td>
<td>20</td>
<td>110</td>
<td>0.03</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Potamogeton sp.</td>
<td>0.10E+00</td>
<td>16</td>
<td>118</td>
<td>0.03</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.005</td>
</tr>
<tr>
<td>Vallisneria sp.</td>
<td>0.30E+00</td>
<td>20</td>
<td>125</td>
<td>0.03</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.005</td>
</tr>
</tbody>
</table>

**Producer populations**

<table>
<thead>
<tr>
<th></th>
<th>B&lt;sub&gt;i&lt;/sub&gt; (gC/m&lt;sup&gt;2&lt;/sup&gt;)</th>
<th>T&lt;sub&gt;i&lt;/sub&gt; (°C)</th>
<th>I&lt;sub&gt;i&lt;/sub&gt; (E/m&lt;sup&gt;2&lt;/sup&gt;/d)</th>
<th>P&lt;sub&gt;max&lt;/sub&gt; (1/d)</th>
<th>snk (1/d)</th>
<th>K&lt;sub&gt;p&lt;/sub&gt; (μgP/L)K&lt;sub&gt;n&lt;/sub&gt; (μgN/L)K&lt;sub&gt;si&lt;/sub&gt; (μgSi/L)</th>
<th>resp (1/d)</th>
</tr>
</thead>
</table>

**Consumer populations**

<table>
<thead>
<tr>
<th></th>
<th>B&lt;sub&gt;i&lt;/sub&gt; (gC/m&lt;sup&gt;2&lt;/sup&gt;)</th>
<th>T&lt;sub&gt;i&lt;/sub&gt; (°C)</th>
<th>C&lt;sub&gt;max&lt;/sub&gt; (1/d)</th>
<th>rsda (1/d)</th>
<th>T&lt;sub&gt;r&lt;/sub&gt; (°C)</th>
<th>R&lt;sub&gt;max&lt;/sub&gt; (1/d)</th>
<th>u (1/d)</th>
<th>cm (1/d)</th>
</tr>
</thead>
</table>

* Producer parameter definitions: B<sub>i</sub> = initial biomass of primary producer population; T<sub>i</sub> = temperature for optimal growth; I<sub>i</sub> = light saturation intensity; P<sub>max</sub> = maximum growth rate; snk = sinking rate (phytoplankton only); K<sub>p</sub> = Michaelis-Menten half-saturation constant for inorganic phosphorus; K<sub>n</sub> = Michaelis-Menten half-saturation constant for inorganic nitrogen; K<sub>si</sub> = Michaelis-Menten half-saturation constant for silica dioxide; resp = dark respiration rate.

* Consumer parameter definitions: B<sub>i</sub> = initial biomass of consumer population; T<sub>i</sub> = water temperature for maximum feeding rate; C<sub>max</sub> = maximum feeding rate; rsda = specific dynamic action (fish only); T<sub>r</sub> = water temperature for maximum respiration rate; R<sub>max</sub> = maximum respiration rate; u = excretion rate; cm = natural mortality rate.
prey

predation as a normalized product of predator and prey bio-

comotion costs, prey preferences, prey assimilation, and tem-

terature-dependent decomposition process; bacteria pop-

created, or egested. The egested fraction is remineralized by a

food consumed by each population is either assimilated, ex-

a handling efficiency for predator

respiration - natural mortality - (specific dynamic action) - predation

or

\[
\frac{dB_i}{dt} = \sum Cm_i \left( h(T) \cdot w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_j \right) \\
+ \left( B_i + \sum w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_j \right) \\
- r_i \cdot h(T) - (u_i + f_i + m_i + rsda_i) \\
- \sum Cm_i \left( h(T) \cdot w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_j \right) \\
+ \left( B_i + \sum w_{ij} \cdot a_{ij} \cdot h_{ij} \cdot B_j \right)
\]

where

- \( B_i \) = the biomass of consumer population \( i \) (gC/m²),
- \( Cm_i \) = the maximum rate of consumption (1/d),
- \( h(T) \) = the temperature dependence of consumption (unitless),
- \( w_{ij} \) = the preference of consumer \( i \) for prey \( j \) (unitless),
- \( a_{ij} \) = the assimilation efficiency for consumer \( i \) and prey \( j \) (unitless),
- \( h_{ij} \) = the handling efficiency (unitless),
- \( r_i \) = the respiration rate for population \( i \) (1/d),
- \( u_i \) = the excretion rate for population \( i \) (1/d),
- \( f_i \) = the egestion rate for population \( i \) (1/d),
- \( m_i \) = the mortality rate for population \( i \) (1/d), and
- \( rsda_i \) = the specific dynamic action that applies to fish only (1/d).

Modeled consumer populations are distinguished by their population-specific rates of feeding, respiration, excretion, locomotion costs, prey preferences, prey assimilation, and temperatures for maximum feeding and respiration.

The consumption term in Equation 8 calculates grazing or predation as a normalized product of predator and prey biomass [26,30] as modified by the preference of predator \( i \) for prey \( j \) (\( w_{ij} \)), the assimilation of prey \( j \) by predator \( i \) (\( a_{ij} \)), and a handling efficiency for predator \( i \) consuming prey \( j \) (\( h_{ij} \)). The food consumed by each population is either assimilated, excreted, or egested. The egested fraction is remineralized by a temperature-dependent decomposition process; bacteria populations are not explicitly modeled. Recycled nutrients are added to the dissolved nutrient pools and assuming a constant C:N:P stoichiometry for plant and animal organic matter. The mathematical nature of the consumption term introduces a density dependence in the overall production of consumer populations in the CASM [30]. At low predator abundances, the biomass of the available predator determines the flux of ingested material into the predator populations. As the predator biomass increases, the flux becomes increasingly determined by the biomass of the prey. Such density dependence can influence the response of individual populations and complex food webs to pesticide exposure in the CASM.

**Temperature dependence.** The effects of water temperature (\( T \) [°C]) on the rates of photosynthesis, consumption, and respiration was formulated using the following equation [31,32]:

\[
h(T) = V \cdot \exp(x(1 - V))
\]

where \( V = (T_m - T) / (T_m - T_o) \). \( T_m \) defines an upper lethal temperature specified for each population and process rate; \( T_o \) specifies the temperature at which the maximum rate (i.e., photosynthesis, respiration, feeding) is observed for each population. The value of \( x \) in Equation 9 is a nonlinear scalar of the ln \( Q_{10} (T_m - T_o) \), where the value of \( Q_{10} = 2.0 \).

**Mass balance.** An overall mass-balance approach was used to develop the CASM. New carbon fixed through photosynthesis by plants remains in the form of plant biomass, is passed up through the food web, enters the particulate organic matter pool (where it might again enter the food web, be decomposed, or accumulate). Consumer biomass exists as standing crop biomass, enters the food web, enters the particulate organic matter pool (where it is also subject to further passages through the food web, is decomposed, or accumulates).

Nutrient inputs to the dissolved inorganic pools in the modeled aquatic ecosystem are removed from solution in relation to the rate of primary production according to an assumed stoichiometry. If the primary production demand for nutrients exceeds the available supply, nutrients are allocated in relation to the relative demand expressed by each population of plants so that nutrient mass remains conserved in the system. Similarly, stoichiometric ratios are used to return nutrients to the dissolved inorganic pools as the result of excretion by consumers and remineralization by decomposers.

**Input parameters for a regional aquatic ecosystem.** The physical, chemical, biological, and ecological characteristics that define the aquatic systems of interest are specified by site-specific data. These data can be obtained from field studies or a literature search for the regional aquatic system of interest.

**Bioenergetics parameters.** The population identities of primary producers and consumers that define the food web for the regional ecosystem of interest (e.g., Central Florida lake) are specified on input. These data also include the bioenergetics-based parameters that determine the rates of growth for each model population. The populations and growth parameters for a generalized Central Florida, USA, lake are presented in Table 3. The populations were identified as being representative species of potential interest or concern in these kinds of systems. The population-specific growth parameters were derived from the technical literature for each species or for related species.

**Food web relations.** The regional aquatic ecosystem is also characterized by grazing and predator-prey interactions. Additional data were developed to define the relative preference (or availability) of each potential food or prey species for each modeled consumer population (\( w_{ij} \)). In addition, the assimilation efficiency (\( a_{ij} \)) for each feeding interrelation was estimated.
Environmental forcing functions. Daily changes in modeled population sizes are influenced by the physical and chemical environment defined for each aquatic ecosystem. Surface light intensity (i.e., irradiance) and water temperature define the physical environment. Concentrations of dissolved inorganic nitrogen, phosphorus, and silica along with dissolved and particulate organic matter describe the chemical environment. Daily values of water temperature, light intensity, and inorganic nutrient loadings were provided to the model for the southeastern lake, a series of pulsed inputs was constructed as the exposure scenario for the CASM simulations. Diquat dibromide was applied to the modeled lake every 6 weeks during the exposure scenario for the CASM simulations. Diquat dibromide was applied to the modeled lake every 6 weeks during the one-year simulation. The highest simulated 90th-percentile, 96-h, time-weighed mean exposure concentration of diquat dibromide (0.0263 mg/L) demonstrated no direct toxic effects on the population with simulations of chronic exposure to concentrations of diquat dibromide at concentrations for daily changes in exposure concentration. The effects factors selected independently from their respective distributions and in relation to the specified daily values of diquat dibromide exposure. Each simulation represented one modeled ecosystem response to an exposure scenario. These CASM results were then used to estimate the probability of observing a 10, 20, 30,..., to 100% reduction in total production integrated over a single year, as well as the probability of a 10% or greater increase in production for each model population. The risk from each magnitude of effect was calculated as the frequency of simulations in which the effect was observed. The modeled precision in estimating risk was 0.01 (i.e., 1/100 simulations). The selected precision of 0.01, though arbitrary, will likely prove to be more precise than risk estimates derived from field observations. This frequentist approach to risk characterization is consistent with quantitative risk analysis as applied in other disciplines [38].

RISK ESTIMATION AND CHARACTERIZATION

The three differently scaled and differently structured ecological risk-assessment models produced results that were consistent in their characterization of risks posed by diquat dibromide.

Daphnia IOM

The IOM produced time series of the lipid and the structural components of Daphnia for the zero-exposure simulation (i.e., reference) and the two exposure scenarios (Tables 4 and 5). The referenced simulations demonstrate the dynamics of these model components in the absence of exposure to diquat dibromide. These time-varying changes in lipid and structural biomass reflect the underlying biological and ecological processes that determine the pattern of growth for the individual Daphnia. Comparisons of the reference Daphnia IOM simulation with simulations of chronic exposure to concentrations of 0.0263 mg diquat cation/L demonstrated no direct toxic effect on the average lipid content of the Daphnia (Table 4). Exceedingly small reductions in lipid content resulted from the exposure to 0.048 mg diquat cation/L. Similarly, comparisons of the reference Daphnia IOM simulation with simulations of chronic exposure to diquat dibromide at concentra-
Table 4. Modeled average *Daphnia* lipid content (μg) for reference individual-oriented model simulation and simulations using diquat cation

<table>
<thead>
<tr>
<th>Time (d)</th>
<th>Reference</th>
<th>0.0263 mg diquat cation/L</th>
<th>0.048 mg diquat cation/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>50.7091</td>
<td>50.7091</td>
<td>50.7091</td>
</tr>
<tr>
<td>5</td>
<td>60.8088</td>
<td>60.8088</td>
<td>60.8080</td>
</tr>
<tr>
<td>10</td>
<td>64.0881</td>
<td>64.0881</td>
<td>64.0869</td>
</tr>
<tr>
<td>15</td>
<td>29.6869</td>
<td>29.6869</td>
<td>29.6864</td>
</tr>
<tr>
<td>20</td>
<td>29.7533</td>
<td>29.7533</td>
<td>29.7529</td>
</tr>
<tr>
<td>25</td>
<td>34.4938</td>
<td>34.4938</td>
<td>34.4934</td>
</tr>
<tr>
<td>30</td>
<td>35.0797</td>
<td>35.0797</td>
<td>35.0792</td>
</tr>
<tr>
<td>35</td>
<td>43.3129</td>
<td>43.3129</td>
<td>43.3123</td>
</tr>
<tr>
<td>40</td>
<td>50.9507</td>
<td>50.9507</td>
<td>50.9499</td>
</tr>
<tr>
<td>45</td>
<td>56.3859</td>
<td>56.3859</td>
<td>56.3850</td>
</tr>
<tr>
<td>50</td>
<td>7.14804</td>
<td>7.14808</td>
<td>7.14799</td>
</tr>
</tbody>
</table>

Table 5. Modeled average structural biomass of *Daphnia* (μg) for reference individual-oriented model simulation and simulations using diquat cation

<table>
<thead>
<tr>
<th>Time (d)</th>
<th>Reference</th>
<th>0.0263 mg diquat cation/L</th>
<th>0.048 mg diquat cation/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>9.76486</td>
<td>9.76486</td>
<td>9.76486</td>
</tr>
<tr>
<td>5</td>
<td>11.3453</td>
<td>11.3453</td>
<td>11.3451</td>
</tr>
<tr>
<td>10</td>
<td>11.8443</td>
<td>11.8443</td>
<td>11.8441</td>
</tr>
<tr>
<td>15</td>
<td>5.62087</td>
<td>5.62087</td>
<td>5.62079</td>
</tr>
<tr>
<td>20</td>
<td>6.31845</td>
<td>6.31845</td>
<td>6.31838</td>
</tr>
<tr>
<td>25</td>
<td>7.21963</td>
<td>7.21963</td>
<td>7.21955</td>
</tr>
<tr>
<td>30</td>
<td>7.11835</td>
<td>7.11835</td>
<td>7.11826</td>
</tr>
<tr>
<td>35</td>
<td>8.57471</td>
<td>8.57471</td>
<td>8.57459</td>
</tr>
<tr>
<td>40</td>
<td>9.79059</td>
<td>9.79059</td>
<td>9.79045</td>
</tr>
<tr>
<td>45</td>
<td>10.6426</td>
<td>10.6426</td>
<td>10.6424</td>
</tr>
<tr>
<td>50</td>
<td>7.14804</td>
<td>7.14808</td>
<td>7.14799</td>
</tr>
</tbody>
</table>

tions of 0.0263 mg diquat cation/L demonstrated no direct toxic effect on the structure of the *Daphnia* population, though small reductions were evident at 0.048 mg diquat cation/L (Table 5). These results, based on a detailed, process-level model for individual growth, suggest that realistic scenarios of diquat dibromide application pose minimal ecological risk to the structural biomass or the lipid content of *Daphnia* [27].

**Bluegill sunfish demographic model**

Figure 4 illustrates an annual projection of the modeled bluegill sunfish population in the absence of exposure to diquat dibromide. After an initial increase, the population is projected to decrease by approximately one order of magnitude. The values defined by the median population size and its confidence intervals provide a reference for comparing the potential impacts of exposing this model population to diquat dibromide.

A combination of the maximum 96-h, time-weighted mean concentration from the EXAMSII lake scenario simulations (0.0263 mg diquat cation/L) and the exposure:response functions developed for the bluegill sunfish produced very small changes (0.00–0.04%) in bluegill survivorship, fecundity, and growth. Previous experience with this model and small parameter perturbations of similar magnitude indicated that it was not necessary to perform the model simulations. Simulations based on these small changes in the bluegill demographic model would project population changes within the confidence interval of the reference simulations. In other words, the effect of an exposure concentration of 0.0263 mg diquat cation/L or lower would have been negligible using the demographic model population for bluegill sunfish. Simulations using the model would confirm that a probability of even a 10% reduction in bluegill population size because of the maximum anticipated exposure to diquat dibromide would be essentially zero.

**CASM**

Results of the CASM simulations of repeated diquat dibromide applications to a generic Central Florida, USA, lake also indicated minimal ecological risks to fish and other aquatic populations. All modeled estimates of risk were zero, except for total annual phytoplankton production; the model estimated a probability of 0.85 that total annual phytoplankton production would decrease by 10% compared with the reference simulation. This result is not entirely surprising, because diquat dibromide is an herbicide. However, the risk of a 20% decline in phytoplankton production was zero for these simulations. Increased mortality or reduced growth of rooted aquatic plants was not observed in these simulations, though diquat dibromide has been used effectively to control nuisance plant growth. Even so, exposures resulting from the direct spraying of macrophytes would be intentionally greater than the water-column exposures used in these simulations. Direct application of diquat dibromide to CASM macrophytes was not modeled.

To examine further the efficacy of using the CASM to estimate ecological risks, additional simulations were performed in which the diquat dibromide exposure concentrations were systematically increased by 10-, 25-, 50-, 75-, and 100-fold. The resulting risk estimates are summarized for phytoplankton in Figure 5 and for benthic invertebrates in Figure 6. Risks remained essentially zero for other model populations even at the highest exposure concentration. Figure 5 illustrates the relationship between the potential magnitude of the simulated impact on phytoplankton with increased exposure to diquat dibromide. The model results that describe risk versus magnitude of impact are approximately parallel with those of increased exposure. This pattern, based on previous experience using the CASM [26], suggests that the impacts on production result mainly from an increase in the direct toxic effects on phytoplankton. Importantly, the results demonstrate that the...
CASMs methodology can simulate toxic effects and corresponding nonzero estimates of risk.

In contrast to phytoplankton, the risks posed by diquat dibromide to modeled benthic invertebrates (including filter-feeders) illustrate a change in the toxicological and ecological processes that determine risk for this functional guild as the exposure concentrations increase (Fig. 6). Risks estimated from the 25-, 50-, and 75-fold exposure scenarios imply direct toxic effects; however, the 100-fold exposure scenario demonstrates the combined direct toxic response and reduced availability of their phytoplankton food resource. The CASM methodology, which is similar to that described previously [27], also can address direct and indirect toxic effects in characterizing ecological risk.

**Discussion**

To be useful in ecological risk assessment, ecological models must have, at minimum, an ecological structure (e.g., populations, trophic interactions, abiotic features) relevant to the pesticide-assessment process, spatial-temporal scales compatible with the fate and effects of pesticides and pesticide management, mathematic linkages that permit inputs of exposure concentrations to be translated into the ecological effects of concern (e.g., mortality, reproductive impairment, reduced growth), and some demonstration of model analysis and evaluation [39].

Intelligent use of ecological models in developing a set of approaches for assessing the risks from pesticides requires an understanding of the possible limitations of these models. Each model presented in this sequential assessment of diquat dibromide corresponds with a particular ecological and mathematical viewpoint. Each model also offers certain advantages afforded by its particular representation of essentially the same natural system: a lake or a pond exposed to diquat dibromide. Understanding the strengths and limitations of each modeling approach might facilitate effective use of the different ecological models in risk assessment or, at least, point out an appropriate level of ecological complexity and corresponding ecological models for specific assessments.

**IOMs**

Despite the *Daphnia* model used in this study showing no difference between the reference simulation and the simulations with diquat dibromide, the modeling exercise demonstrated that an IOM can be implemented for estimating the ecological risks associated with use of pesticides. Toxic chemicals often directly interfere with biochemical reactions, and individual organisms are conveniently scaled for an initial assessment of toxic effects. The IOM considers the biology and the growth dynamics of the exposed organism, which are important in determining how a toxicant affects the modeled individual. Effects on individuals can then be used to extrapolate population-level impacts or risk. Again, in this model, individual biomass (or individuals aggregated into a population) is described in units of lipid or structure. Given a more toxic pesticide or higher exposures to diquat dibromide, simulations using the IOM would demonstrate which *Daphnia* cohorts might be at risk and estimate the risks for a population of exposed individuals.

Models of individual organisms may be particularly useful for assessing the effects of pesticides on small populations of threatened or endangered species, species of recognized socioeconomic importance, or species that are ecologically important (e.g., keystone predators, bioindicators). One promising avenue in developing risk-characterization methods for pesticides would be using IOMs to derive parameter distributions for aggregated population models. For example, the collective deaths of individuals exposed to pesticides as calculated using an IOM could be used to estimate age- or size-specific mortality rates or even survivorship parameters in an aggregated population model [40].

One possible limitation of IOMs is that a population-level equation is applied to many state variables that are called individual organisms but that, in fact, merely represent merely a highly disaggregated population model. That an emergent property of an IOM so constructed has a dynamic similar to that produced by an aggregated (i.e., single state variable) model constructed for the same population should be unsurprising. Another limitation of IOMs is in deriving parameter values that are truly individualistic for large numbers of individual organisms [41].

Despite their limitations, IOMs could be developed for organisms subjected to pesticide exposure, particularly birds and smaller mammals. For example, to provide a more realistic risk assessment, an IOM was developed to simulate the intake of contaminated food by diving ducks for varying conditions, such as weather, water depth, food dispersion, and the size and digestibility of food [42].
Demographic models

The modified demographic model for the bluegill sunfish demonstrated the potential usefulness of this approach to assess population-level ecological risks. In addition to models developed for fish, demographic population models have also been developed for other species of terrestrial plants and animals [17]. Emlen [43] has reviewed terrestrial population models that might be used in ecological risk assessment, and models for trees and understory vegetation have been summarized by Caswell [17]. Saether and Haagenrud [44] developed a demographic model to examine the effects of age and body size on the reproductive output of the moose (Alces alces), and their model might be adapted to assess the risks for larger mammals potentially exposed to pesticides. Taylor [45] modeled the dynamics of insect populations, and this model might be adapted to examine pesticide impacts on non-target soil insects. Finally, Lande [46] constructed a demographic model for the northern spotted owl (Strix occidentalis caurina) to address the environmental effects of logging; this model might be adapted to examine pesticide effects on the spotted owl or similar bird species.

The demographic modeling approach affords several advantages in assessing ecological risks. Importantly, these models can be developed in a stochastic framework to provide probabilistic estimates of populations changes when characterizing risks, examining recovery [25], or exploring the implications of population-management alternatives. In addition, the demographic modeling calculations are relatively straightforward and make fewer computational demands than the IOM or the CASM. Another advantage of the demographic approach is that the effects of pesticides on known or suspected sensitive age or size classes can be modeled explicitly, and the implications of these sensitive classes on projections of future population sizes can then be assessed.

The primary constraint in adapting demographic models for risk characterization is deriving the exposure (or dose)-response functions relating exposure to changes in the demographic parameters (i.e., survivorship, fecundity) that determine the modeled population dynamics. A similar limitation in developing this method for pesticides is the typically steep slope of the exposure-response functions. Another possible constraint is the annual time step typical of the models developed for fish. It may prove to be impractical to collect the data necessary to reduce the time step to the scales relevant to pulsed pesticide exposures (e.g., hours, days). Our study demonstrated that a combination of calibration and field data can be used to fill in the data gaps that are necessary in developing models that require finer time scales. Many of the limitations of demographic models have been addressed, and this modeling approach has been useful in ecological risk estimation [20].

Community and ecosystem models

The CASM application demonstrated that the ecological risks posed by pesticides can be estimated as the probability of a specified percentage decrease in producer or consumer community-production dynamics. Ecological risks can also be assessed as changes in community structure, biodiversity, total ecosystem production and respiration, or nutrient cycling using richly structured ecological models such as the CASM. Because the CASM is embedded in a self-contained Monte Carlo framework, the results are directly applicable to probabilistic assessments of risk. Sensitivity analyses used to identify key sources of variability in model performance are also readily performed with these kinds of models [27,47].

In addition to the number of parameters and inputs required, other limitations of the CASM include the potential sensitivity of results to the mapping of limited toxicity data onto model populations [29], that toxic effects are based on concentrations of dissolved pesticide and not on pesticide in sediments or actually bioaccumulated, that chemical fate processes are not included in the model, the daily time scale of the model, and that the model addresses only one toxic chemical per simulation.

Model evaluation

This study demonstrated the potential for using differently structured and scaled ecological models to characterize ecological risks. The extent to which this potential translates into actual practice depends, in no small part, on demonstrating the accuracy and reliability of these (and other) ecological models. However, the lack of detailed experimental or monitoring data that describe the ecological impacts of diquat dibromide under conditions consistent with the assumptions particular to each modeling approach precludes detailed, quantitative model evaluations. Nevertheless, at least circumstantial evidence supports continued examination of these modeling approaches for application in risk assessment. The individual-oriented modeling approach has provided accurate characterization of the growth dynamics of individual Daphnia [8,9]. Demographic models of fish populations have been useful in assessing the impacts of physical and chemical stressors on the production dynamics of fish populations [20]. The bioenergetics-based approach underlying the CASM has provided accurate estimates of the impacts from phenolic compounds on populations of primary producers, zooplankton, and fish [27]. The Littoral Enclosure Risk Assessment model, which derives from the CASM and uses the same calculus for estimating ecological production dynamics and for characterizing toxic effects, has accurately estimated the ecological impacts of other pesticides [47,48]. The CASM has also simulated the basic production dynamics of phytoplankton, zooplankton, benthic invertebrates, and fish within one order of magnitude of measured values collated for aquatic ecosystems in Quebec [49]. At the same time, the limitations of these modeling approaches are recognized, and future efforts should delineate those ecological conditions and pesticide types for which the models accurately and reliably estimate ecological impacts and risks.

CONCLUSIONS

Three fundamentally different modeling approaches were used to estimate the ecological risks of diquat dibromide. The ecological models implemented for this assessment add to the set of strictly empirical methods [1] and provide more ecologically realistic, process-oriented methods for estimating the ecological risks from pesticides. As reported previously [1], results of the ecological model simulations consistently indicated that diquat dibromide poses minimal ecological risk in exposure scenarios resulting from the recommended application rates. Initially, the realization that all these assessment tools produced estimates of minimal risk for the very low exposure concentrations of diquat dibromide made us question the need to perform the assessment and the value of this pesticide as a demonstration case study. On further consideration, however, we concluded that establishing the ability to characterize minimal risk was a priori no less important than pre-
senting a case study based on a more toxic compound. In addition, repeating the model simulations (e.g., CASM) with sufficiently high exposure concentrations demonstrated that the method can produce correspondingly higher estimates of risk.

Ecological models will likely play an increasingly important role in characterizing ecological risks given the diminished resources available to support laboratory and field studies. Therefore, it remains important to rigorously examine and evaluate previously developed ecological modeling approaches to determine their relevance for characterizing ecological risks. The issue is not model complexity or population versus ecosystem models but identifying the necessary and sufficient model structure and processes that produce useful and reliable estimates for specific risk assessments and management decisions based on risk.

Acknowledgement—This study was funded by Zeneca Ag Products (Wilmington, DE, USA).

REFERENCES


