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Evaluating the new PWC modeling scenarios for ecological risk assessment

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1 Introduction

A modeling scenario is a set of predefined input parameters for one or more models. For the ecological risk assessment (ERA) on pesticides in surface water, a modeling scenario consists of meteorological conditions, landscape and soil characteristics, and template receiving water body. A well-developed modeling scenario establishes the foundation for estimating the exposure potentials of a pesticide product, and provides consistent comparisons between different chemicals, products, and use patterns. The integration of modeling scenarios with a pesticide modeling system also significantly simplifies the risk assessment procedures, so that users can focus on the pesticide-specific data including physicochemical properties and pesticide application schemes.

The Office of Pesticide Programs (OPP) of the U.S. Environmental Protection Agency (USEPA) has been using a set of crop scenarios in the modeling of pesticide applications to land surfaces and subsequent transport to and fate in water bodies. The active model for aquatic risk assessment is the Pesticide in Water Calculator (PWC) (Young, 2020), so the crop scenarios are also referred to as "PWC scenarios". The early development of the scenarios was started in the early 2000s with the release of an integrated modeling system "PRZM/EXAMS" or PE by OPP. The scenarios were later extended with the model applications to ERA and the Endangered Species Act (ESA), such as the modeling studies for organophosphate pesticides and California red-legged frogs. While OPP keeps evolving the simulation engines and integrated modeling system, the same set of crop scenarios have been used in all generations of the OPP models, including PE, Surface Water Concentration Calculator (Fry et al., 2013), and multiple versions of PWC.

In April 2023, OPP released a new version of PWC scenarios on its webpage of models for pesticide risk assessment (USEPA, 2023). Technical details on the development and selection of the new scenarios have been documented earlier in the regulatory docket EPA-HQ-OPP-2020-0279 for "Pesticide Drinking Water Assessment Improvements". The new scenarios were originally developed for drinking water assessment in a USEPA index reservoir (USEPA, 2020), and thus coded as "dw_scenarios_v4" (drinking water scenarios version 4). Later, OPP decided to use them for both drinking water and ecological assessments (USEPA, 2023). At the same time, the previous scenarios were removed from the OPP website. However, this does not mean that modeling results with the previous scenarios are immediately rejected by OPP. As of this study, most of the modeling studies for ecological risk assessment and biological evaluation posted by OPP after April 2023 were still based on the previous scenarios.

Since 2012, the Surface Water Protection Program (SWPP) of the California Department of Pesticide Regulation (DPR) has been developing the Pesticide Regulation Evaluation Model (PREM) for more consistent and transparent evaluation of pesticide registration packages for surface water protection (Luo and Deng, 2012a, b). PREM models various pesticide use patterns for ERA in surface water, including agricultural, aquatic, rice, urban/residential, and right-of-way applications. For agricultural applications, PREM currently uses the same scenarios as in PWC. Both the previous and new PWC scenarios are incorporated in the latest version of PREM, version 6 (Luo et al., 2024a).

The development and evaluation of the new PWC scenarios for drinking water assessment have been well documented (USEPA, 2020). However, their applications on ERA have not been evaluated. The objective of this study is to compare the previous and new PWC scenarios for ERAs on pesticides in surface water. The motivations and questions expected to be answered in this study include:

1) The new scenarios were developed based on the long-term average EDWCs (estimated drinking water concentrations) in the water column of an index reservoir, i.e., 54-year averages also called "cancer concentrations" (USEPA, 2019, 2020). Their modeling capability and performance for ERA are not evaluated. An ERA is based on estimated environmental concentrations (EECs) in both the water column and benthic region of a USEPA farm pond, with a much shorter averaging period than the cancer concentrations for drinking water, e.g., daily average EECs for acute assessment or 21-d average EECs for chronic assessment.
2) OPP only compared the new and previous scenarios for "corn" based on the cancer concentrations predicted in selected regions in the U.S. In addition, the corn scenarios in California were not included in the comparison.
3) For almost of the tested scenarios for corn, the OPP's modeling results indicated that the previous scenarios would rank well above the 90^{th} percentile at which the new scenarios were determined. This finding suggested that, compared to the previous scenarios, the new scenarios would generally underestimate the cancer concentrations from pesticides used for corn. Therefore, several questions arise for their applications in ERA: (a) What are the major causes for the underestimation? (b) Is this conclusion also valid for EECs in the water column and benthic region? (c) If so, what are the levels of overestimation (or more generally, the relative changes) for the EECs predicted by the new vs. previous scenarios? (d) What about the corn scenarios in California (not tested by OPP), and what about use patterns other than corn (not tested by OPP)?

4) OPP provided the new scenarios for 15 crop groups in California. Do they sufficiently cover the pesticide use patterns actively evaluated by SWPP? And which scenario should be assigned to each use pattern?
5) Unlike the previous scenarios which are independent of chemical properties, OPP created three new scenarios for each crop group based on the KOC value of the pesticide to be modeled: set "A" for KOC<100, "B" for KOC from 100 to 3000, and "C" for KOC>3000 L/kg[OC]. For the modeling results, therefore, it is anticipated to observe abrupt changes by slightly increasing the KOC value from 99 to 101, or from 2999 to 3001 L/kg[OC]. Given the uncertainty on the reported KOC values for a pesticide, the modeling results and associated regulatory decisions may not be consistent.

Review of the development documents suggests that the methodology for creating and selecting the new scenarios is scientifically solid. Based on a spatially distributed modeling approach and quantitative ranking of modeling results, the parameterization processes in the new scenarios are more consistent and transparent compared to the previous version, and expected to generate more realistic results reflecting aquatic concentrations and their spatial distributions. This study is not to question or challenge the new scenarios, but to evaluate their applications and implications on ERAs, which are not sufficiently demonstrated by the OPP. The results herein are anticipated to be used to justify or adjust the ERA modeling results during the transition period from the previous PWC scenarios to the new version.

2 Overview of the PWC modeling scenarios

2.1 Data in a PWC scenario (both previous and new PWC versions)

The new PWC scenarios updated input values, but maintained the general structure of included information as in the previous scenarios. A scenario consists of two categories of input variables: spatial data (weather, crop, land surface, and soil) and non-spatial or system data (simulation period and default modeling options). The system data are independent of crop or geographic location. For example, the runoff extraction efficiency was set as 0.266 for all previous scenarios or 0.19 for all new scenarios, regardless of crops and regions. Spatial data (such as landscape characteristics, soil properties, and weather stations), however, are specific to the crop and location to be modeled. More details are provided in the next two sub-sections for the spatial data in the previous and new scenarios.

2.2 The previous PWC scenarios

The previous PWC scenarios were developed for major crops or land uses in each state. For example, the previous scenarios for California include 20 crops and some non-crop scenarios (impervious surface, residential and commercial turf, weeds, nursery, forestry, and rangeland).

Spatial data in the previous scenarios were developed from the representative production area of the corresponding crop and state, and metadata have been provided to explain the parameterization processes for each scenario. For example, the field representing the almond production in California was located in San Joaquin County in the Central Valley (USEPA, 2004). The weather data were taken from Sacramento Executive Airport, which was the nearby National Weather Service station available at the time of development. The GIS data layers, local expert opinions, and survey results were incorporated in the determination of soil and crop parameters.

2.3 The new PWC scenarios

The new PWC scenarios were developed based on a more systematical approach. Gridded GIS layers were aligned for weather, soil, and cropland data, and combined to create the *field scenarios* in a spatially continuous way over the U.S. at a resolution of 30×30 m^2. The 255 crops in the cropland data layer (CDL) were aggregated into 17 crop groups for modeling. Additional crop parameters, such as the growth calendar and irrigation, were determined from the spatial databases and survey results from the U.S. Department of Agriculture (USDA) and OPP in-house development (USEPA, 2007). The source codes for the automated field scenario generation have been posted in GitHub ("USEPA/opp-efed-scenarios").

The resulting field scenarios were further grouped by crop in each hydrologic region represented by a 2-digit hydrologic unit code (HUC2). Note that not all 17 crop groups were modeled for a hydrologic region. For example, soybean and sugarcane were not considered in the California hydrologic region (HUC2 = 18, or "r18"). The field scenarios for each crop/region were ranked by the PWC-predicted cancer concentrations (54-year overall average EDWCs), and the one which represented the 90th percentile was selected as the final PWC scenario for the corresponding crop and region (USEPA, 2020). OPP repeated this selection process by modeling three hypothetical chemicals with KOC values of 10, 1,000, and 10,000 L/kg[OC], so there are three scenarios for each crop/region:

1) Scenario set "A", developed based on the hypothetical chemical with KOC=10 L/kg[OC], and proposed to be used for pesticides with KOC below 100 L/kg[OC];
2) Scenario set "B", developed with KOC=1,000 L/kg[OC], and used for KOC = 100 to 3,000 L/kg[OC]; and
3) Scenario set "C", developed with KOC=10,000 L/kg[OC], and used for KOC over 3,000 L/kg[OC].

The cutoff KOC values of 100 and 3,000 L/kg[OC] are equal to or close to the geometric medians between the modeled KOCs: geometric median (10, 1,000) = 100 and geometric median (1,000, 10,000) = 3,162.

For the California hydrologic region ("r18"), specifically, there are 15 crop groups (Table 1) and 45 (=15×3) scenarios in total. Some discrepancies are observed by comparing the development methodology (USEPA, 2020) and the final released products. For example, Christmas trees were not considered a separate crop in the development but combined with evergreen orchards. In addition, pasture/forage was originally proposed for another OPP model (the Spatial Aquatic Model), but finally produced as one of the PWC scenarios.

Table 1. The new PWC scenarios for California and associated crops indexed by the cropland data layer (CDL) crop identifier

New PWC scenario	CDL crop and code
“Christmas Trees”	Christmas Trees (70)
“Corn”	Corn (1), Pop or Orn Corn (13)
“Cotton”	Cotton (2)
“Hay all”	Alfalfa (36), Clover/Wildflowers (58), Vetch (224). Other Hay/Non-Alfalfa (37), Switchgrass (60), Mint (14)
“Orchard deciduous”	Apples (68), Pears (77), Cherries (66), Nectarines (218), Peaches (67), Apricots (223), Plums (220), Prunes (210), Almonds (75), Pecans (74), Pistachios (204), Walnuts (76), Pomegranates (217), Other Tree Crops (71)
“Orchard evergreen”	Citrus (72), Oranges (212), Olives (211)
“Other grains or corn”	Sorghum (4), Millet (29)
“Pasture or forage”	Pasture/Grass (62), Grass/Pasture (176), Sod/Grass Seed (59)
“Row or field crop”	Sunflower (6), Peanuts (10), Tobacco (11), Sugarbeets (41)
“Small fruit trellised”	Grapes (69), Caneberries (55), Blueberries (242), Hops (56)
“Small grains”	Barley (21), Buckwheat, (39), Oats (28), Other Small Grains (25), Rye (27), Speltz (30), Triticale (205), Camelina (38), Canola (31), Flaxseed (32), Rapeseed (34), Safflower (33), Mustard (35)
“Vegetable commodity”	Dry Beans (42), Potatoes (43), Sweet Potatoes (46), Onions (49), Peas (53), Chick Peas (51), Lentils (52)
“Vegetable fresh or processing market”	Sweet Corn (12), Broccoli (214), Cabbage (243), Cauliflower (244), Garlic (208), Cantaloupes (209), Honeydew Melons (213), Watermelons (48), Cucumbers (50), Gourds (249), Pumpkins (229), Squash (222), Tomatoes (54), Eggplants (248), Peppers (216), Greens (219), Lettuce (227), Carrots (206), Radishes (246), Turnips (247), Asparagus (207), Celery (245), Herbs (57), Misc Vegs & Fruits (47), Strawberries (221)
“Wheat spring”	Durum Wheat (22), Spring Wheat (23)
“Wheat winter”	Winter Wheat (24)

2.4 Linking the PWC scenarios with the use patterns modeled in PREM

Table 2 links the new PWC scenarios to the agricultural use patterns in PREM. See Table 1 for more information on the individual crops and the designated scenarios. There are both “wheat spring” and “wheat winter” in the new scenarios (Table 1), and “wheat winter” is used here to be consistent with the previous scenario “CAWheat” which was developed based on winter wheat. In summary, the 19 agricultural high-risk use patterns are modeled by only nine new scenarios. Some use patterns will share the same new scenario. For example, broccoli (representing brassica "cole" leafy vegetables), lettuce (leafy vegetables), strawberry, and tomato will use the same scenario for “Vegetable fresh or processing market” (Table 2). Strawberry is included here, even though it is a small fruit, as its production practices are similar to fresh market vegetables (Hansel et al., 2020).

Table 2. Relating the new PWC scenarios to the agricultural use patterns in PREM

Agricultural high-risk use patterns in PREM	Previous scenarios	New scenarios
Alfalfa	“CAalfalfa”	“Hay all”
Broccoli	“CAColeCrop”	“Vegetable fresh or processing market”
Citrus	“CAcitrus”	“Orchard evergreen”
Corn	“CAcorn”	“Corn”
Cotton	“CAcotton”	“Cotton”
Grains	“CAWheat”	“Wheat winter”
Grape	“CAgrapes”	“Small fruit trellised”
Lettuce	“CAlettuce”	“Vegetable fresh or processing market”
Row crops	“CARowCrop”	“Row or field crop”
Stone fruits	“CAfruit”	“Orchard deciduous”
Strawberry	“CAStrawberry”	“Vegetable fresh or processing market”
Sugar beet	“CAsugarbeet”	“Row or field crop”
Tomato	“CAtomato”	“Vegetable fresh or processing market”
Tree nuts	“CAalmond”	“Orchard deciduous”

3 Methodology for evaluating the new PWC scenarios

Following the OPP configurations in the development of the new scenarios (USEPA, 2020), the following sets of hypothetical chemicals were used in this study:

1) Three hypothetical chemicals with persistent half-lives (HLs = 180 days) and KOC values of 10, 1,000, and 10,000 L/kg[OC], i.e., the same chemicals used by OPP. The three chemicals were the primary test agents in this study for evaluating the new scenarios and comparing with the previous one.
2) Three hypothetical chemicals with *quick dissipation* (HLs = 5 days) and KOC values of 10, 1,000, and 10,000 L/kg[OC]. While the new scenarios were developed based on long-term (54 years) averages of EDWCs, this study focused on the daily EECs for ERA. Therefore, additional evaluations on the chemicals with short half-lives were proposed.
3) Hypothetical chemicals with persistent half-lives (180 days) and KOC values varying from 10 to 10,000 L/kg[OC].

The chemical sets (1) and (2) were the primary test agents in this study for evaluating the new scenarios and comparing the results with the previous ones. Modeling results are presented in Sections 4.1 and 4.2. The set (3) chemicals were used to evaluate the three scenarios (“A”, “B”, and “C”) for each crop (results in Section 4.3).

Other modeling settings were also consistent with the OPP. Pesticide applications were modeled as continued daily applications over a long period (50 days starting from the crop emergence which is predefined in each scenario). The single application rate was set to be 0.1 kg/ha. Note that the application rate is proportional to the predicted pesticide loads and EECs, and will be cancelled when calculating the relative changes for modeling results from the previous vs. new scenarios.

In the PWC, spray drift is independent of crop scenarios. Since this study was focused on pesticide runoff and erosion predicted with the previous and new scenarios, spray drift was not modeled, i.e., application efficient = 100% and spray drift fraction = 0.

For ERA, the USEPA pond was modeled as the receiving water body. Modeling results were summarized as the 1-in-10-year daily average EEC in the water column (EEC[w], μg/L) and in the benthic region (as pore-water concentration, EEC[b], μg/L). The same form of EECs were used by SWPP for registration evaluation (Luo, 2017). The relative changes of the EECs were reported for each pair of previous and new scenarios (the same equation is applied to both EEC[w] and EEC[b]):

$$\Delta EEC = \frac{EEC(new)}{EEC(previous)} - 1$$

4 Results and discussions

4.1 Relative changes on EECs

The six hypothetical chemicals (three with persistent HLs and three with quick dissipation) were modeled with the 14 high-risk use patterns (Table 2) parameterized by the previous and new scenarios. For each chemical and use pattern, the model results with the new scenario were compared to those with the old one, and the relative changes on the EECs in the water column (ΔEEC[w]) and in the benthic region (ΔEEC[b]) are reported in Table 3. There are 168 values representing the relative changes. Most (145 out of 168, or 86%) of the ΔEECs are negative values, indicating that the EECs decrease by switching from the previous scenario to the new scenario. The relative changes range from -99.6% (ΔEEC[b], row crops, KOC=10,000 L/kg[OC], HL=5 days) to 441.4% (ΔEEC[b], tomato, KOC=10,000 L/kg[OC], HL=180 days). The median of all ΔEEC is -70.7%, suggesting that the EECs with the new scenarios are about 30% of those with the previous scenarios.

Table 3. Relative changes on the EEC in the water column (ΔEEC[w]) and in the benthic region (ΔEEC[b]) predicted by the new vs. old scenarios. A negative value indicates a decrease on EEC by switching from the previous scenario to the new one. KOC values are in the unit of L/kg[OC].

(a) Hypothetical chemicals with persistent half-lives

Use pattern	KOC=10 (scenario "A")		KOC=1,000 ("B")		KOC=10,000 ("C")	
	ΔEEC[w]	ΔEEC[b]	ΔEEC[w]	ΔEEC[b]	ΔEEC[w]	ΔEEC[b]
Alfalfa	66.1%	89.6%	-96.5%	-95.3%	-27.6%	-27.8%
Broccoli	-87.0%	-86.1%	-79.6%	-81.6%	-36.8%	-47.8%
Citrus	-80.0%	-76.0%	35.0%	52.1%	51.1%	53.7%
Corn	17.8%	27.3%	-94.0%	-93.8%	-57.5%	-71.9%
Cotton	-71.5%	-63.9%	-30.5%	-23.8%	21.7%	-36.0%
Grains	-11.9%	-10.4%	-70.8%	-74.9%	-70.5%	-83.4%
Grape	-71.2%	-69.5%	-61.7%	-60.5%	-17.5%	-10.4%
Lettuce	-82.0%	-80.2%	-71.1%	-72.3%	-24.6%	-31.3%
Row crops	-78.4%	-79.9%	-88.8%	-90.0%	-38.2%	-18.5%
Stone fruits	-62.9%	-65.0%	-50.7%	-54.6%	-28.7%	4.0%
Strawberry	-85.5%	-83.9%	-86.7%	-84.3%	-33.3%	-28.3%
Sugar beet	-72.1%	-72.7%	-72.2%	-72.2%	-24.1%	54.7%
Tomato	-43.5%	-24.2%	-21.1%	11.4%	278.5%	441.4%
Tree nuts	-62.8%	-65.5%	-66.1%	-73.6%	-53.9%	-65.1%

(b) Hypothetical chemicals with quick dissipation

Use pattern	KOC=10 (scenario "A")		KOC=1,000 ("B")		KOC=10,000 ("C")	
	ΔEEC[w]	ΔEEC[b]	ΔEEC[w]	ΔEEC[b]	ΔEEC[w]	ΔEEC[b]
Alfalfa	195.8%	107.1%	-98.7%	-98.7%	47.7%	-4.8%
Broccoli	-90.5%	-92.2%	-94.7%	-97.2%	-82.3%	-92.0%
Citrus	-85.8%	-81.0%	-4.9%	14.1%	-49.5%	-46.2%
Corn	-6.2%	-18.8%	-98.7%	-99.2%	-83.3%	-91.0%
Cotton	-89.3%	-86.3%	-84.3%	-77.8%	11.6%	18.8%
Grains	45.1%	-15.3%	-58.4%	-80.5%	-71.1%	-88.5%
Grape	-77.7%	-79.3%	-66.5%	-71.9%	-86.3%	-88.8%
Lettuce	-82.2%	-84.3%	-92.9%	-96.1%	-77.6%	-88.9%
Row crops	-83.7%	-89.3%	-81.0%	-86.2%	-99.4%	-99.6%
Stone fruits	-67.6%	-68.2%	-46.8%	-44.1%	-57.1%	-60.6%
Strawberry	-86.1%	-89.3%	-96.4%	-97.9%	-71.9%	-84.8%
Sugar beet	-79.6%	-86.4%	-57.1%	-67.0%	-99.3%	-99.5%
Tomato	-60.6%	-56.1%	-82.1%	-84.0%	30.1%	16.7%
Tree nuts	-59.5%	-67.2%	-63.9%	-66.0%	-70.3%	-78.0%

The individual ΔEEC values reported in Table 3 are summarized as median values over the modeled pesticide use patterns and chemicals (Table 4).

Table 4. Median ΔEECs over the modeled use patterns and chemicals. KOC values are in the unit of L/kg[OC].

Hypothetical chemicals	KOC=10	KOC=1,000	KOC=10,000
Persistent half-lives	-70.4%	-72.2%	-28.1%
Quick dissipation	-79.5%	-81.6	-77.8%
All	-71.8%	-74.3%	-47.0%

Although most of the modeling results show decreasing EECs, positive ΔEEC values are observed for 8 out of 14 modeled use patterns. The other six use patterns (broccoli, grape, lettuce, row crops, strawberry, and tree nuts) are associated with consistent underestimations by comparing the EECs in both water column [w] and benthic region [b] predicted by the new scenarios compared to the previous ones.

Table 5. Modeled use patterns with positive ΔEECs (i.e., increased EECs by changing from the previous to new scenarios). KOC values are in the unit of L/kg[OC].

Hypothetical chemicals	KOC=10	KOC=1,000	KOC=10,000
Persistent half-lives	Alfalfa, corn	Citrus, tomato (EEC[b] only)	Citrus, cotton (EEC[w]), stone fruits (EEC[b]), sugar beet (EEC[b]), tomato
Quick dissipation	Alfalfa, grains (EEC[w])	Citrus (EEC[b])	Alfalfa (EEC[w]), cotton, tomato
All	Alfalfa, corn, grains (EEC[w])	Citrus, tomato (EEC[b] only)	Alfalfa (EEC[w]), citrus, cotton, stone fruits (EEC[b]), sugar beet (EEC[b]), tomato

4.2 General mechanisms for the relative changes

The relative changes presented in Table 3 are primarily attributed to three factors: [1] surface runoff generation, [2] soil erosion, and [3] application timing (scheduled according to the predefined emergence date). The three factors are also interrelated with each other. For example, more surface runoff will increase soil erosion, and application timing determines the pesticide amounts accumulated in the soil available for runoff extraction especially during the winter rain season in California.

Compared to the previous ones, the new scenarios are generally associated with lower runoff potential, evaluated as the ratio between the predicted surface runoff vs. total incoming water (precipitation and irrigation). This is also confirmed by the lower curve number (CN) values used in the new scenarios. The PWC predicts surface runoff based on the Soil Conservation Service (SCS) curve number method (USDA, 1985), and a lower CN value indicates more permeable soil and less runoff generation.

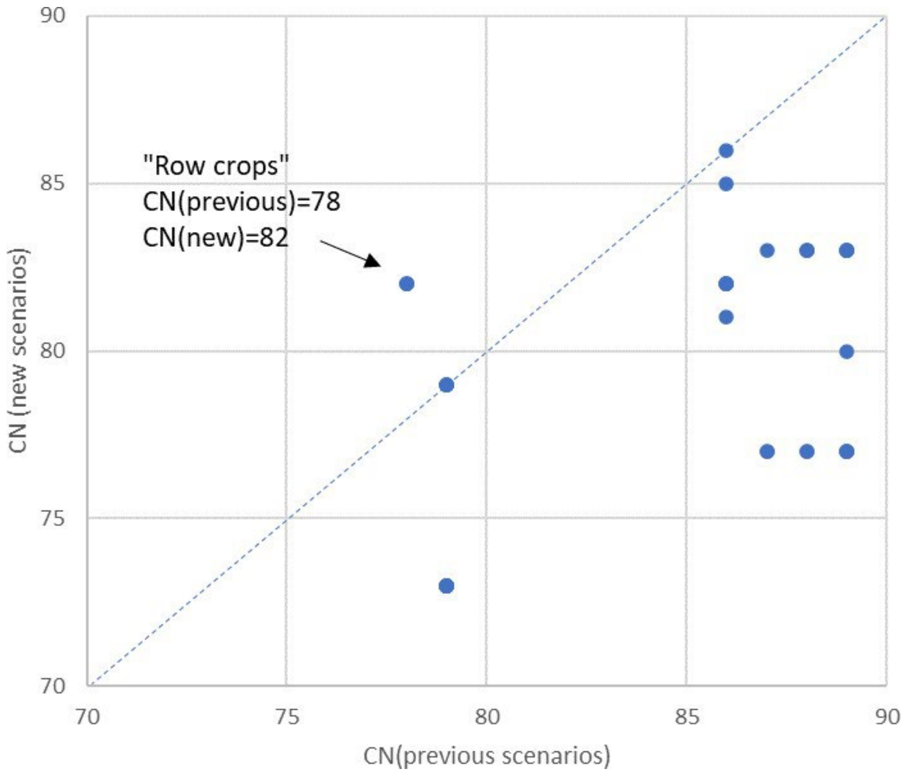


Figure 1. Curve number (CN) values during growing seasons in the previous vs. new scenarios evaluated in this study (Table 2). A data point under the 1:1 line indicates that the new scenario has lower CN values than the previous one.

Figure 1 compares the CN values during growing seasons in the previous and new scenarios paired for the pesticide use patterns modeled in this study. There are 42 data points, and some of them overlap each other. Most of the new scenarios have lower (34 out of 42) or the same (5) CN values relative to the corresponding previous ones. Only for the use pattern of row crops, the three new scenarios, i.e., "Row or field crop-r18-A", "-B", and "-C", have higher CNs than the previous scenario "CARowCrop" (Figure 1).

The median precipitation over the modeled new scenarios is 33.1 cm/year (ranging from 7.3 to 52.0), higher than that in the previous scenarios (median = 27.0 cm/year). The relative changes of precipitation range from -86% (scenario "B" for row crops) to 259% (scenario "B" for citrus). However, the change of precipitation is not a factor sufficiently explaining the relative changes predicted for the model predictions presented in Table 3. As shown in Figure 2, for most of the scenarios (in the dashed circle), the predicted EEC[w] are decreased regardless of the precipitation change.

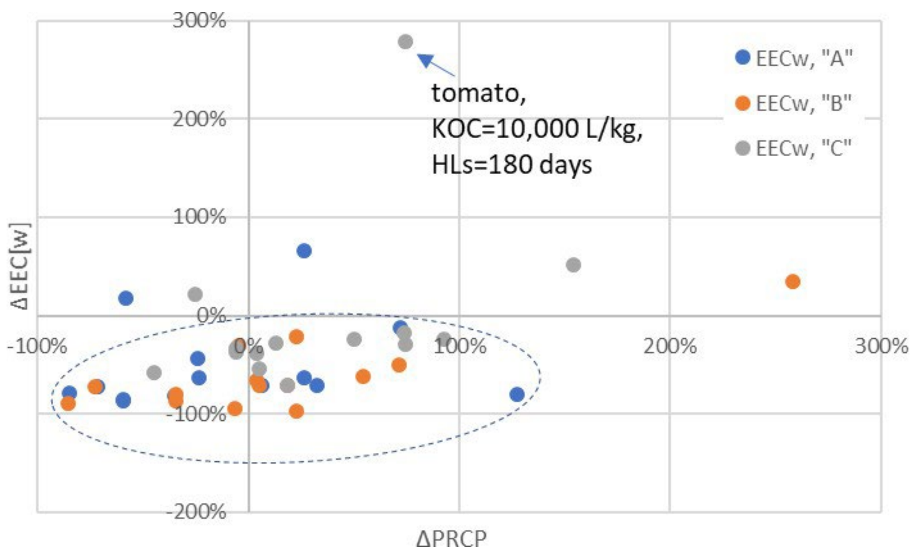


Figure 2. Relative changes of the predicted pesticide loads (y-axis, ΔEEC[w], values from Table 3) and the precipitation (x-axis, ΔPRCP) between the new vs. previous scenarios. Inside the dashed circle are the data points with negative ΔEEC[w] values.

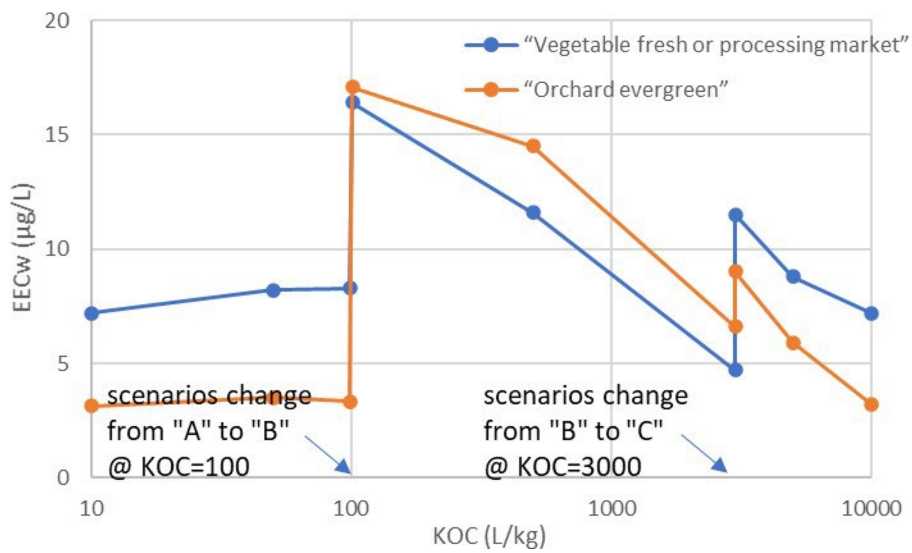
For the persistent chemicals (modeled with a half-life of 180 days), their accumulated residues in the soils would be subject to surface runoff and soil erosion during the winter rain season in California. Modeling for tomato with a high KOC is an example for this condition (Figure 2), which results in significantly higher EECs with the new scenario compared to the previous one (ΔEEC[w] = 279%, and ΔEEC[b] = 441%, Table 3). Further investigations on the daily model outputs indicate that the high EECs are contributed by the winter fallow season. The new scenario ("Vegetable fresh or processing market-r18-C", Table 2) is characterized with later applications (the first application at emergence on July 23, compared to March 1 in the previous scenario "CAtomato") and higher soil erodibility (USLE-C = 0.611 during the fallow season, 444% higher than the average value in the previous scenario).

4.3 Investigations on the three scenarios ("A", "B", and "C") for each crop

For each crop and hydrologic region, OPP developed three scenarios that represent high runoff (scenario "A" developed with KOC=10 L/kg[OC]), high erosion ("C" with KOC=10,000 L/kg[OC]), and mixed ("B" with KOC=1,000 L/kg[OC]) conditions. OPP proposed to use the scenario "A" for chemicals with KOC<100 L/kg[OC], "B" for KOC = 100 to 3,000 L/kg[OC], and "C" for KOC>3,000 L/kg[OC]. Due to the great uncertainty on the reported KOC values, a chemical with a KOC around 100 may be modeled by the scenarios of "A" or "B", and a chemical with a KOC around 3,000 may be modeled by the scenarios of "B" or "C". Therefore, the uncertainty on KOC values and the associated use of modeling scenarios could result in significantly different modeling results for the same chemical and application schemes.

Additional evaluations were conducted by modeling a hypothetical chemical with KOC values varying from 10 to 10,000 L/kg[OC]. Two set of new scenarios were selected for demonstration: "Vegetable fresh or processing market" and "Orchard evergreen" (Figure 3). Significant changes are observed for EECs with KOC changing from 99 to 101 L/kg[OC] (scenario from "A" to "B") and from 2,999 to 3,001 L/kg[OC] (scenario from "B" to "C"). The magnitudes of change are dependent on the scenarios and persistence. With the change of the "Orchard evergreen" scenarios from "A" to "B", for example, the EEC[w] increases by 413% and 466%, respectively for the hypothetical chemical with persistent half-lives (Figure 3a) and quick dissipation (Figure 3b). Slightly decreased EECs are observed for the hypothetical chemicals with quick dissipation (Figure 3b), -1.0% with the change of the "Vegetable fresh or processing market" scenarios from "A" to "B" and -26.6% with the change of the "Orchard evergreen" scenarios from "B" to "C". For chemicals with a model input of KOC around the critical values of 100 or 3,000 L/kg[OC], therefore, additional efforts are required to ensure the EECs are not underestimated.

(a) Hypothetical chemicals with persistent half-lives



(b) Hypothetical chemicals with quick dissipation

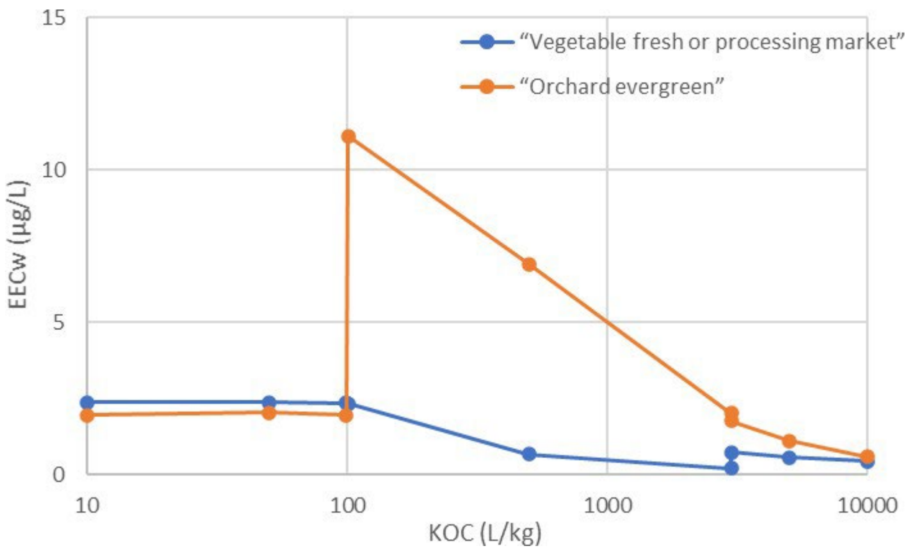


Figure 3. EECw (µg/L) vs. KOC from 10 to 10,000 modeled for hypothetical chemicals with (a) persistent half-lives and (b) quick dissipation under new scenarios.

5 Conclusions and recommendations

This study is the first of its kind to systematically evaluate the new PWC scenarios for aquatic ERA. The model output variables for evaluation were selected as the 1-in-10-year daily average EECs in the water column and benthic region. The 14 high-risk agricultural use patterns identified by SWPP were modeled by both the new and previous scenarios in California for hypothetical chemicals with various half-lives and KOC values. The modeling results (Table 3) are presented as the relative changes of EECs for 168 paired simulations (= 14 use patterns, 3 KOCs, 2 half-lives, and 2 environmental media of water column and benthic region).

The modeling results indicate that, for most of the case studies (145 out of 128, or 86%), the predicted pesticide loads and EECs by the new scenarios are lower than those by the previous scenarios. This finding is consistent with OPP's evaluations (USEPA, 2020) for cancer concentrations in drinking water assessment with the selected "corn" scenarios across the U.S. In this study, the median relative changes on EECs are about -70% for low and intermediate KOC, and about -50% for high KOC over all modeled scenarios and chemicals (Table 4).

Specifically for the registration evaluations by SWPP, the generally decreased EECs with the new scenarios may affect the model-based recommendations for agricultural uses under certain conditions. An SWPP evaluation is based on a risk quotient (RQ, calculated as the ratio between EEC and acute toxicity endpoint) in comparison with the level of concern at 0.5. For the previous RQs (i.e., RQs modeled by the previous scenarios) above but close to 0.5, the new modeling results could be lower than 0.5 for some use patterns and chemicals. To further evaluate the potential effects, the new scenarios were applied to all SWPP registration evaluations posted from 2011 to 2024 with the reported RQs > 0.5 for non-rice agricultural uses. Results showed that the new modeling results did not change the previous model-based recommendations.

The new scenarios are only developed for selected production crops, but not for non-agricultural uses as in the previous scenarios, including impervious surfaces, residential lawns, weeds (for right-of-way applications), outdoor nursery, non-irrigated rangeland, forest, and turf areas (golf courses, parks, sod farms, and recreational fields) (Luo et al., 2024b). Before the corresponding new scenarios become available, the removal of all previous scenarios from the OPP modeling website for PWC will hinder the processes for pesticide registration evaluation and post-use risk assessment. At this time, if SWPP decides to switch to and *only* use the new scenarios, PREM will lose about half of its designated modeling capabilities in terms of pesticide use patterns to be evaluated.

Therefore, the recommendation for SWPP registration evaluation is to keep using the previous PWC scenarios before a complete package of the new scenarios is released to model all relevant use patterns in PREM. Meanwhile, the currently available new scenarios will be considered for the evaluations on pesticide uses for terrestrial crops (Table 2). For those use patterns, if the predicted RQs by the previous scenarios are above 0.5, the evaluation could be refined with the new scenarios. This only accounts for a small percentage (less than 2%) of the total registration reviews by SWPP based on the previous evaluations in the last ten years, so it will not substantially change the well-established evaluation processes.

OPP created three scenarios for each crop group, and significant changes on the EECs were predicted when KOC changed across the critical values of 100 and 3,000 (Figure 3). There are some concerns related to this issue:

1) The reported KOC values are usually associated with great uncertainties, but only their statistical summary (e.g., the median) as a single value is used for modeling.
2) For multiple active ingredients in a pesticide product, they may be associated with KOC values in different ranges and thus evaluated by different scenarios representing inconsistent weather and landscape settings.
3) Similarly, a parent compound and its degradates may have to be modeled with different scenarios.

If the accepted KOC values are in a range across the critical value of 100 or 3,000, therefore, additional modeling efforts with the new scenarios may be needed to ensure that the potential exposure is not underestimated because of the input KOC value and assigned scenario. See Appendix I for the proposed additional evaluations.

Finally, this study is only aimed at comparing the two versions of PWC scenarios in a relative way, not including validations with monitoring data. It’s noteworthy that the previous scenarios have been widely used by regulatory agencies and scientific communities in the past decades. Many of these studies conducted model validation by comparing the model predictions (with the previous scenarios) to measured data in surface water. By switching to the new scenarios, it’s anticipated to generate lower concentration results, which would challenge the previously established modeling results and associated implications, recommendations, and regulatory decisions. Studies to be impacted include most of the previous USPEA's ERAs where the predicted EECs with the previous scenarios were justified by the monitoring data, such as the ERAs on neonicotinoids (USEPA, 2016a) and pyrethroids (USEPA, 2016b). Results with the new scenarios may not be able to meet the previously used criteria that the EECs and the 90th percentile monitored concentrations should be "*within one order of magnitude difference of each other*" (USEPA, 2016b).

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Appendix I. Additional evaluations on the uncertainty of input KOC values

The standard registration evaluation is based on the median KOC value (Luo et al., 2024a). For evaluating the new PWC scenarios, additional evaluations are needed if the median and upper confidence interval of KOC values are located in two different KOC zones, where the zones are defined in the new PWC scenarios as: "A" for KOC < 100, "B" for 100 ≤ KOC ≤ 3000, and "C" for KOC>3000 L/kg[OC]. The accepted KOC values are first sorted in ascending order, and their upper confidence interval is determined as (1) if the number of input KOC values is less than 8 (n<8), the upper interval is the maximum KOC value (i.e., the last number in the sorted data or i = n); (2) if n≥8, use Table 6 to determine the upper confidence interval. For example, for 20 values of KOC (n=20), the upper interval is the 15th order statistic.

Table 6. Confidence intervals for the median by sample size (n) and associated confidence coefficients (P)

n	(i,n+1-i)	$P(Y_i<m<Y_{n+1-i})$
<8	(1,n)	NA
8	(2,7)	0.9286
9	(2,8)	0.9610
10	(2,9)	0.9786
11	(3,9)	0.9346
12	(3,10)	0.9614
13	(3,11)	0.9776
14	(4,11)	0.9426
15	(4,12)	0.9648
16	(5,12)	0.9232
17	(5,13)	0.9510
18	(5,14)	0.9692
19	(6,14)	0.9364
20	(6,15)	0.9586

Note: the confidence coefficient (probability) is calculated based on binomial distribution: $P(Y_i<m<Y_{n+1-i}) = P(W<n+1-i) - P(W<i)$, where n is the sample size.

Based on the zones for the median and upper confidence interval of KOC, additional evaluations are specified in Table 7. The highest RQ results between the standard (median KOC) and additional (critical KOCs, Table 7) evaluations will be used for ecological risk assessment.

Table 7. Additional evaluations if the median and upper confidence intervals of KOCs are in different KOC zones. KOC values in the unit of L/kg[OC].

Median KOC	Upper confidence interval KOC	Additional evaluation
Zone "A" (KOC < 100)	Zone "B" (100 ≤ KOC ≤ 3000) or "C" (KOC>3000)	Evaluation with KOC = 101
Zone "B"	Zone "C"	Evaluation with KOC = 3001

The proposed additional modeling has minimum impact on the registration evaluation by SWPP. Based on the previous evaluations, only a small number of active ingredients have their median and upper confidence interval of KOC in different KOC zones, and some of these pesticides are not registered for use on terrestrial crops. Further investigation indicates that, in the last five years, none of the new active ingredients evaluated by SWPP need additional modeling due to the uncertainty in the submitted KOC values.