Development of Groundwater Pesticide Exposure Modeling Scenarios for Vulnerable Spring and Winter Wheat-Growing Areas

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ABSTRACT
Wheat crops and the major wheat-growing regions of the United States are not included in the 6 crop- and region-specific scenarios developed by the US Environmental Protection Agency (USEPA) for exposure modeling with the Pesticide Root Zone Model conceptualized for groundwater (PRZM-GW). The present work augments the current scenarios by defining appropriately vulnerable PRZM-GW scenarios for high-producing spring and winter wheat-growing regions that are appropriate for use in refined pesticide exposure assessments. Initial screening-level modeling was conducted for all wheat areas across the contiguous United States as defined by multiple years of the Cropland Data Layer land-use data set. Soil, weather, groundwater temperature, evaporation depth, and crop growth and management practices were characterized for each wheat area from publicly and nationally available data sets and converted to input parameters for PRZM. Approximately 150,000 unique combinations of weather, soil, and input parameters were simulated with PRZM for an herbicide applied for postemergence weed control in wheat. The resulting postbreakthrough average herbicide concentrations in a theoretical shallow aquifer were ranked to identify states with the largest regions of relatively vulnerable wheat areas. For these states, input parameters resulting in near 90th percentile postbreakthrough average concentrations corresponding to significant wheat areas with shallow depth to groundwater formed the basis for 4 new spring wheat scenarios and 4 new winter wheat scenarios to be used in PRZM-GW simulations. Spring wheat scenarios were identified in North Dakota, Montana, Washington, and Texas. Winter wheat scenarios were identified in Oklahoma, Texas, Kansas, and Colorado. Compared to the USEPA’s original 6 scenarios, postbreakthrough average herbicide concentrations in the new scenarios were lower than all but Florida Potato and Georgia Coastal Peanuts of the original scenarios and better represented regions dominated by wheat crops. Int. Environ. Assess. Manag. 2017;13:992–1006. © 2017 The Authors. Integrated Environmental Assessment and Management published by Wiley Periodicals, Inc. on behalf of Society of Environmental Toxicology & Chemistry (SETAC)

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INTRODUCTION
The US Environmental Protection Agency (USEPA) Office of Pesticide Programs (OPP) has used the Pesticide Root Zone Model for groundwater (PRZM-GW) to estimate pesticide concentrations in groundwater for drinking water exposure assessments since 2012 as part of the North American Free Trade Agreement (NAFTA) to develop a unified groundwater modeling protocol (HC and USEPA 2012). The PRZM-GW is a 1-dimensional finite difference solution to the fate and vertical transport of agricultural pesticides though the crop root zone. In the PRZM-GW conceptual model, pesticides are applied to a field of uniform crop with negligible runoff and erosion and maximum infiltration of precipitation and irrigation water. The field sits atop a standardized soil profile and shallow unconfined aquifer with a 100-cm drinking water well screen (Figure 1). Average groundwater concentrations in the well screen zone simulated on a daily time step provide the estimated concentrations used in exposure and risk assessments.

The USEPA created 6 regional parameterizations of the spatially varying soil-, weather-, and crop-related input parameters to PRZM-GW in regions considered to be vulnerable to groundwater contamination (OPP 2015). The 6 regional parameterizations or standard scenarios (OPP 2013), shown in Figure 2, are

1) Florida Citrus,
2) Florida Potato,
3) Wisconsin Corn,
4) Georgia Peanuts,
5) North Carolina Cotton, and
6) Delmarva Sweet Corn.

The USEPA guidance on the implementation of PRZM-GW in pesticide exposure assessments recommends that, for Tier 1 screening-level modeling, all 6 standard scenarios should be simulated. However, if the standard scenarios do not represent the pesticide use, Tier 2 refined modeling, which includes development of representative scenarios, should be conducted (OPP 2015).

The 6 standard PRZM-GW scenarios, located exclusively in the eastern and midwestern United States, represent a small subset of labeled uses for pesticides and their associated geographic regions. No grain crops are included in the standard scenarios. Most notably wheat, which is predominantly grown in the Central West and West, is not represented. Wheat-growing areas according to the most recent 5 y (2009–2013) of the Cropland Data Layer (NASS 2009–2013) available at the time of analysis are compared to the counties represented by the standard scenarios in Figure 2. The minimal overlap of wheat in these counties demonstrates that exposure assessments based on the current scenarios would not be representative of the environmental and agronomic conditions of pesticides specifically used on wheat crops. Therefore, representative wheat scenarios need to be developed to characterize potential groundwater exposure at wheat sites.

The USEPA guidance on the selection of scenario locations states that the areas should be vulnerable to groundwater contamination, including areas where the depth to groundwater is shallow (<100 ft) and where the potential for leaching and persistence is high (USEPA and HC 2012a). However, there is no specific process outlined in the guidance for defining the vulnerable locations. In the past, USEPA has used a US Geological Survey (USGS) national study of groundwater vulnerable to nitrate leaching (Nolan and Hitt 2006) to justify the location of the existing standard scenarios (OPP 2015), but nitrate vulnerability is not an ideal surrogate for pesticides. Sources of N include fertilizer as well as soil organic matter, which may have a different spatial and temporal pattern than pesticide applications. A systematic, reproducible method is needed to define the location and corresponding model input parameters of PRZM-GW crop scenarios so that more pesticide and crop uses can be evaluated within USEPA’s existing framework for pesticide exposure refinement (Tier 2 modeling).

The goal of the present paper is to define both appropriately vulnerable PRZM-GW scenarios that represent major spring and winter wheat–growing regions of the United States and to present a systematic method for their development. The approach uses publicly and nationally available soil, crop, and groundwater data sets to identify locations where 3 criteria co-occur: high (85th–95th percentile) estimated groundwater concentrations, shallow groundwater depth (overlap with shallowest principal aquifer), and largest wheat acreage. Extensive site-specific exposure modeling is conducted to achieve a comprehensive map of estimated herbicide concentrations in groundwater for the nation. Model results combined with crop and groundwater depth information provide the basis for 8 new wheat scenarios (4 winter, 4 spring) for PRZM-GW to be used in exposure assessments.

The process for identifying wheat scenario locations and extracting model input parameters relevant to those locations is outlined in the Methods section. The resulting 8 scenarios and their corresponding modeled groundwater concentrations are summarized in the Results section. Comparisons of estimated herbicide concentrations for the new wheat scenarios and for the 6 standard scenarios are presented in the Discussion section.

**METHODS**

The key to developing representative PRZM-GW scenarios for wheat was determining appropriate sites from which to extract the spatially dependent model input parameters. The USEPA guidance on scenario location selection is limited, stating only that locations should be in regions that are vulnerable to groundwater contamination without providing...
methodology or metrics for how to determine vulnerable locations. The approach outlined here used a combination of exposure modeling and spatial analysis in a 2-step process (Figure 3) to define appropriate sites. The first step involved extensive modeling using PRZM-GW to screen for regions (states) with both high estimated herbicide concentrations in groundwater and high wheat acreage. From within these vulnerable states, the sites near shallow groundwater wells were selected as representative scenarios and model parameters were finalized, in the second step. Details on the modeling conducted and data evaluated in each step follow.

Screening simulations

Screening modeling with a nonvolatile, moderately mobile (soil–water partition coefficient, $K_{oc}$, 144.4 mL/g), and slightly degradable (stable hydrolysis, 126-d surface soil degradation half-life) herbicide was conducted with PRZM-GW for potential wheat-growing soils and weather conditions throughout the nation to create a national map of potential groundwater herbicide concentrations. Wheat sites in all counties in 8 high-priority wheat states (Minnesota, North Dakota, South Dakota, Wyoming, Montana, Washington, Oregon, Idaho) and additional counties outside of those states with greater than 5000 wheat acres grown annually were included in the modeling (Figure 2). Annual wheat acreage by county was determined from the 2012 Census of Agriculture (NASS 2014). The specific locations of wheat sites in those counties were defined by the footprint of spring, winter, and durum wheat classes plus other crop classes double-cropped with wheat found in the Cropland Data Layer (CDL) in any year between 2009 and 2013 (NASS 2009–2013) (Figure 2).

Given the wheat footprint described above, subsequent spatial analysis identified unique combinations of soils, weather, and cropping practices that overlapped with the wheat areas. Unique soil–weather–cropping combinations were used to define PRZM-GW input parameter sets or scenarios that were then used in 100-y model simulations to capture temporal variability and to extend the period of time over which breakthrough to the aquifer may be observed for less mobile chemicals. Separate analyses were conducted for spring and winter wheat, which have different typical cropping practices and regions of production. The result was predictions of herbicide concentrations in groundwater from nearly 150 000 PRZM-GW simulations (61 313 spring wheat, 84 978 winter wheat) sampling the wide range of environmental conditions characteristic of wheat-growing areas.

Model parameterization

Vertical profiles of soil parameters were extracted from the Soil Survey Geographic database (SSURGO; NRCS 2012) component and horizon attribute tables. All soil components in map units co-occurring with the wheat footprint described above (Screening simulations, first paragraph) were evaluated. Only soil components with the necessary horizon data to a depth greater than 0.8 m were included in modeling. This avoided extrapolation of soil parameters in the sensitive aerobic degradation zone of the model (0–1 m), thus limiting unnecessary introduction of uncertainty. The SSURGO attributes used in the PRZM-GW parameterization are listed with their corresponding model parameter for an example component in Table 1. The SSURGO horizon data, which may be discretized at varying...
depths and thickness, was standardized to the PRZM-GW conceptual soil profile, shown in Figure 1, using interpolation and depth-weighted averaging. Standardized horizon parameters were calculated based on the proportion of the SSURGO horizon overlapping the PRZM-GW horizon. An example calculation is provided in Table 1. For numerical integration, each PRZM-GW horizon was further discretized, using the same scheme as the USEPA standard scenarios (see Figure 1), with soil parameters constant throughout the horizon. The depth to the shallow aquifer was standardized to 4 m for all screening runs, regardless of the extent of SSURGO component data, to limit the time to chemical breakthrough and provide a standard basis for comparing soil profiles. Not all components had complete attribute data in all horizons. In certain cases, missing data could be estimated or extrapolated from available parameters. Missing sand and clay percentages were estimated if any 2 of sand, clay, and silt percentages were available in the same horizon. Missing wilting point and field capacity data were estimated when sand, clay, organic matter, and bulk density were available using the linear regression equations developed by Rawls et al. (1982) following Method 1 outlined in the PRZM manual using the coefficients in the manual (Suárez 2006, Table 5.23).

Weather data from the Solar and Meteorological Surface Observation Network (SAMSON; CEAM 2006a) climate stations were associated with soil components and wheat areas by combining Thiessen polygons around the stations with SSURGO map units and the wheat crop footprint. Precipitation, evapotranspiration, temperature, wind speed, and solar radiation time series from the SAMSON stations were extended from 30 to 100 y by repeating the original data in 30-y blocks following USEPA procedure. Cropping practices, crop growth, and field conditions that vary regionally were summarized by state for modeling purposes. These characteristics included crop emergence, maturity and harvest timing, pesticide application timing, irrigation, groundwater temperature, and evaporation depth. Emergence, maturity, and harvest dates for wheat were determined from the Usual Planting and Harvesting Dates for US Field Crops report (NASS 1997), discussions with experts, and previous USEPA modeling practices. For spring wheat, emergence, maturity, and harvest dates were varied by state to facilitate modeling variation in the pesticide application dates, which are typically timed relative to emergence. For winter wheat, herbicides are applied in the spring unrelated to the timing of fall emergence. Therefore, regional variations in emergence, maturity, and harvest were not introduced as factors affecting application timing in the modeling. Emergence for spring wheat was assumed to occur 21 d after planting, based on discussions with crop specialists. This value was also within the 5- to 39-d range for 50% wheat seedling emergence predicted by Wang et al. (2009). Spring wheat planting dates by state were selected from the midpoint of the most active planting ranges reported in NASS 1997. Not all states growing spring wheat were included in the usual planting and harvesting table. The planting date selected for states not reported in the table was the average of the reported spring wheat–planting dates. Maturity for spring wheat was assumed to occur 70 d after emergence based on the USEPA North Dakota (ND, spring) wheat standard scenario commonly used to parameterize PRZM for surface water modeling. The spring wheat harvest dates were selected as the midpoints of the most active harvest ranges reported in NASS 1997. For spring wheat–growing states not in the report, harvest was assumed to occur 11 d after maturity, following the timing used in the North Dakota wheat standard scenario. One foliar herbicide application of 0.07 kg a.i./ha was simulated annually 24 d after emergence for spring wheat, based on personal communication with crop specialists.

Emergence for winter wheat was assumed to occur 21 d after planting, the same as for spring wheat. The single winter wheat planting date, October 11, was selected by averaging the midpoint of the most active planting range for all states from NASS 1997. Maturity for winter wheat was assumed to occur 213 d after planting, based on the midpoint of the typical maturity range (200–225 d) for winter wheat in Table 5.9 of the PRZM user manual (Suárez 2006). The winter wheat harvest date of July 8 was determined by
averaging the most active harvest date ranges over all states (NASS 1997). One foliar herbicide application of 0.07 kg a.i./ha was simulated annually on April 1 for winter wheat, based on personal communication with crop specialists (D Porter, Syngenta Crop Protection, personal communication). A complete listing of crop growth and application timing by state and wheat crop is provided in online Supplemental Data Table S1.

Irrigation was simulated in California, Oregon, and Idaho for spring wheat and in California and Oregon for winter wheat, based on personal communications with extension agents, crop profiles (NIFA 2014), and NASS Quick Stats (NASS 2013). The groundwater temperature was calculated by state using an area-weighted average of temperature data mapped in the PRZM user manual (Suárez 2006). These model inputs are summarized in Supplemental Data Table S3.

Additional screening-level modeling parameters were set to conservative default values for all simulations following USEPA PRZM-GW guidance documents (USEPA and HC 2012a, 2012b), previous practices used in USEPA PRZM standard scenarios (CEAM 2006b), and the PRZM user manual (Suárez 2006). These model inputs are summarized in Supplemental Data Table S3.

Given the large number of simulations required to conduct a nationwide vulnerability screen, PRZM modeling was executed at the command line outside of the PRZM-GW graphical user interface (GUI). Python scripts were used to efficiently process simulations in parallel. Python scripts were also used in postprocessing model results to replicate the PRZM-GW GUI calculations for throughputs, breakthrough time, and postbreakthrough average herbicide concentration in the well screen zone. Postbreakthrough average concentrations were the primary model results used to identify vulnerable locations. Postbreakthrough average concentrations were calculated by averaging all daily concentrations in the well screen after pesticide breakthrough to the end of the simulation. “Breakthrough” is defined as the point at which one throughput of the overall soil profile pore volume has infiltrated to the water table, with the postbreakthrough average concentration representing the approximate steady-state average concentration in the top 1 m of the aquifer.

Representative vulnerable PRZM-GW scenarios

Scenario location selection began by identifying the states with the most vulnerable groundwater. The area-weighted sum of the 85th to 95th percentile screening-level postbreakthrough average groundwater concentrations were compared for each state. This metric identified the states that...
produced a large amount of wheat in areas associated with higher potential groundwater concentrations. For example, a state with only a few wheat acres associated with relatively lower groundwater concentrations would have low vulnerability, whereas a state with many wheat acres associated with relatively high groundwater concentrations would have high vulnerability. States with low wheat acreage at high concentrations or high wheat acreage at low concentrations would have moderate vulnerability ranked according to how high and low the wheat acreage and associated concentrations were. An example is shown in Figure 4, comparing the weighted sum (area under the curves) between the 85th and 95th percentile concentrations for Texas, Kansas, Oklahoma, and Colorado winter wheat (top) and Texas, North Dakota, Montana, and Washington spring wheat (bottom). Using this metric, Oklahoma, for example, has more area associated with high concentrations than does Colorado and would therefore be considered a more vulnerable state.

For the top 4 most vulnerable states for spring and winter wheat (total of 8), a single site from screening modeling was selected as the basis for the representative scenario. The screening simulation in each state best satisfying the following criteria was targeted for selection:

- Postbreakthrough average groundwater concentrations near the 90th percentile concentration for the state
- Associated with a shallow groundwater aquifer
- Associated with a large wheat area.

In other words, the representative scenario should exist at the intersection of these criteria. To satisfy the first
requirement, sites with concentrations between the 85th and 95th percentiles were located. From those sites, the sites overlapping the principal shallow aquifer with the shallowest groundwater wells in the state were identified to satisfy the second requirement. Lastly, of the resulting sites in the shallowest aquifer, the one associated with the largest area of wheat was selected as the representative for the state.

Groundwater depths in the principal shallow aquifers were estimated using depth to water-level (feet below land surface) observations from the wells in the USGS Groundwater Daily Data for the Nation (USGS 2015). Of the 6967 groundwater sites with daily data, 3410 sites with depth data from 1985 to present were associated with the shallowest principal aquifers of the conterminous United States (USGS 2003a) by national aquifer code. Shallow principal aquifers were chosen as the basis for groundwater depth in developing new representative scenarios for exposure assessments because they are the uppermost aquifer systems with potential to be used as a source of potable water. The principal aquifer boundaries and water depths at corresponding sites averaged over all years of data are shown in Figure 5. These features were used to find the wheat sites overlapping the aquifer with the shallowest groundwater wells. A subset of groundwater depths in key wheat states is summarized by aquifer in Table 2.

To finalize the representative scenarios, the 4-m screening-level groundwater depth was updated to the overall average depth of the aquifer (final column in Table 2) corresponding to the chosen wheat site. For states without any groundwater sites, for example, Kansas and Montana, data from a neighboring state sharing the same aquifers were used to identify wheat sites and the final groundwater depth.

| State | Principal aquifer name | Nr groundwater monitoring sites | Minimum site depth (m) (avg over all years) | Maximum site depth (m) (avg over all years) | Aquifer depth (m) (avg over all sites and all years) |
|-------|------------------------|--------------------------------|--------------------------------------------|--------------------------------------------|--------------------------------------------------|
| CO    | Colorado Plateaus aquifers | 1                              | 17                                         | 17                                         | 17                                               |
|       | Denver Basin aquifer system | 1                              | 4                                          | 4                                          | 4                                                |
|       | High Plains aquifer      | 4                              | 37                                         | 63                                         | 44                                               |
| ND    | Lower Tertiary aquifers  | 1                              | 5                                          | 5                                          | 5                                                |
| OK    | Ada-Vamoosa aquifer      | 5                              | 2                                          | 48                                         | 26                                               |
|       | Arbuckle-Simpson aquifer | 7                              | 8                                          | 33                                         | 19                                               |
|       | Blaine aquifer           | 10                             | 3                                          | 29                                         | 12                                               |
|       | Central Oklahoma aquifer | 4                              | 25                                         | 88                                         | 52                                               |
|       | Edwards-Trinity aquifer system | 3                          | 1                                          | 24                                         | 11                                               |
|       | High Plains aquifer      | 6                              | 7                                          | 66                                         | 27                                               |
|       | Other rocks aquifers     | 20                             | 0                                          | 28                                         | 6                                                |
|       | Ozark Plateaus aquifer system | 6                        | 5                                          | 110                                        | 41                                               |
|       | Rush Springs aquifer     | 10                             | 3                                          | 35                                         | 18                                               |
| TX    | Coastal lowlands aquifer system | 24                        | 2                                          | 113                                        | 44                                               |
|       | Edwards-Trinity aquifer system | 44                      | 1                                          | 328                                        | 66                                               |
|       | High Plains aquifer      | 12                             | 41                                         | 105                                        | 71                                               |
|       | Rio Grande aquifer system | 2                              | 17                                         | 87                                         | 52                                               |
|       | Seymour aquifer          | 1                              | 13                                         | 13                                         | 13                                               |
|       | Texas coastal uplands aquifer system | 3                      | 10                                         | 81                                         | 45                                               |
| WA    | Columbia Plateau basaltic-rock aquifers | 1                         | 12                                         | 12                                         | 12                                               |
|       | Northern Rocky Mountains Intermontane Basins aquifer systems | 1                         | 30                                         | 30                                         | 30                                               |
|       | Puget Sound aquifer system | 1                              | 8                                          | 8                                          | 8                                                |

Table 2. Summary of groundwater depth by US state and principal shallow aquifer in top vulnerable states

Groundwater depths in the principal shallow aquifers were estimated using depth to water-level (feet below land surface) observations from the wells in the USGS Groundwater Daily Data for the Nation (USGS 2015). Of the 6967 groundwater sites with daily data, 3410 sites with depth data from 1985 to present were associated with the shallowest principal aquifers of the conterminous United States (USGS 2003a) by national aquifer code. Shallow principal aquifers were chosen as the basis for groundwater depth in developing new representative scenarios for exposure assessments because they are the uppermost aquifer systems with potential to be used as a source of potable water. The principal aquifer boundaries and water depths at corresponding sites averaged over all years of data are shown in Figure 5. These features were used to find the wheat sites overlapping the aquifer with the shallowest groundwater wells. A subset of groundwater depths in key wheat states is summarized by aquifer in Table 2.

To finalize the representative scenarios, the 4-m screening-level groundwater depth was updated to the overall average depth of the aquifer (final column in Table 2) corresponding to the chosen wheat site. For states without any groundwater sites, for example, Kansas and Montana, data from a neighboring state sharing the same aquifers were used to identify wheat sites and the final groundwater depth. Because Tier 2 estimated groundwater concentrations are designed to be conservative, representing only the subset of...
the population relying on shallow, private drinking water wells (OPP 2015), the groundwater depth in the final scenarios was limited to no more than 9 m—the maximum depth used in the standard PRZM-GW scenarios. As a last step, the pan evaporation factor was updated from the screening-level default value to a specific value for the representative scenario locations using the Pan Evaporation Correction Factors map from the PRZM user manual (Suárez 2006, Figure 5.9).

RESULTS

Screening simulation results

Groundwater concentrations of the herbicide in screening simulations varied across the nation from 0 \(\mu g/L\) to an absolute nationwide maximum of 41 \(\mu g/L\) for spring wheat and 45 \(\mu g/L\) for winter wheat applications. About 6.2% of spring wheat–growing areas and 3.9% of winter wheat–growing areas did not experience any chemical breakthrough to the water table during the 100-y simulations. The nationwide distributions of groundwater concentrations for spring and winter wheat, graphed in Figure 6, show that concentrations were predicted to be 1 \(\mu g/L\) or less at the majority of wheat sites (>60% for both spring and winter wheat). The area-weighted 90th percentile postbreakthrough average concentrations over all simulations were 2.9 \(\mu g/L\) and 3.2 \(\mu g/L\) for spring and winter wheat, respectively. These concentrations occurred in the latter half of the simulation time period. The area-weighted 90th percentile time to breakthrough over all simulations was 28,600 d (78 y) for spring wheat and 25,600 d (70 y) for winter wheat. The area-weighted 10th percentile time to breakthrough over all simulations was 4600 d (13 y) for spring wheat and 2700 d (7.4 y) for winter wheat.

On the state level, the area-weighted 90th percentile postbreakthrough average herbicide concentrations in groundwater ranged from 0.6 \(\mu g/L\) (NV winter wheat) to 5.2 \(\mu g/L\) (VA spring wheat). The 90th percentile concentration for each state is summarized, along with the acres of wheat harvested according to the 2012 NASS Census of Agriculture (NASS 2014), in Table 3. Several of the more vulnerable states on the basis of concentration alone had some of the lowest harvested wheat acres, indicating that only a small area of groundwater would be exposed at those levels. Relatively higher concentrations occurred in states with wetter weather and/or more vulnerable soil types. The soil hydrologic group was a strong indicator of groundwater concentrations as shown in Figure 6. Although, nationally, there were few sandy, hydrologic group A soils in wheat regions, they resulted most prevalently in groundwater concentrations greater than 5 \(\mu g/L\). The hydrologic group B and C soils most commonly resulted in groundwater concentrations less than 1 \(\mu g/L\).

Representative vulnerable PRZM-GW scenarios

Representative PRZM-GW scenarios were identified for 4 of the top 5 states vulnerable to groundwater contamination (those with high concentrations within the 85th to 95th percentile, over a large area) for both winter and spring wheat. Using the area-weighted sum of screening-level concentrations in the 85th to 95th percentile range for each state (concentration-area integral tabulated in Table 3), the top spring wheat states in order from most to least vulnerable were Texas, North Dakota, Montana, and Washington. Accordingly, the top winter wheat states, in descending order of vulnerability, were Kansas, Texas, Oklahoma, and Colorado. Although North Dakota was also in the top 5 winter wheat states, it was already accounted for in the spring wheat scenarios, so the next most vulnerable state, Colorado, was included for geographic diversity. For the same reason, Washington was included in the spring wheat states instead of Colorado, which was also in the top 5 but already included in the winter wheat scenarios.

Following the criteria of high concentration, shallow groundwater, and large impacted area, the specific sites selected from screening modeling as representative scenarios for the most vulnerable states are presented in Table 4. An example of the selection process is illustrated in Figure 7 for Oklahoma winter wheat. Wheat sites corresponding to the 85th to 95th percentile concentrations (highlighted in red) overlapping the top 3 shallowest aquifers in Oklahoma from Table 2 (Other rocks, Edwards-Trinity aquifer system, and Blaine aquifer) were considered for the representative scenario. The Other rocks classification is given to wide

![Figure 6](image-url)
Table 3. Spring and winter wheat 90th percentile screening modeling groundwater concentrations, harvested wheat acres, and concentration-area integral by US state

| State | 90th percentile concentration (µg/L)a | Harvested acresb | Concentration-area integralc | State | 90th percentile concentration (µg/L)a | Harvested acresb | Concentration-area integralc |
|-------|--------------------------------------|------------------|-------------------------------|-------|--------------------------------------|------------------|-------------------------------|
| VA    | 5.2                                  | 1800             | 231,300                       | ID    | 5.1                                  | 738,400          | 1,254,400                     |
| MI    | 4.7                                  | 300              | 1,029,000                     | VA    | 5.1                                  | 240,200          | 233,100                       |
| WI    | 4.6                                  | 16,300           | 291,400                       | GA    | 5.0                                  | 227,100          | 161,600                       |
| NC    | 4.3                                  | 200              | 749,100                       | COd   | 4.8                                  | 2,167,900        | 2,624,200                     |
| CO    | 4.3                                  | 14,000           | 2,305,200                     | SC    | 4.8                                  | 215,700          | 240,500                       |
| WY    | 3.9                                  | —                | 151,900                       | MI    | 4.5                                  | 538,900          | 998,000                       |
| OR    | 3.7                                  | 123,800          | 636,100                       | WI    | 4.4                                  | 245,300          | 285,500                       |
| WAd   | 3.4                                  | 517,600          | 1,663,900                     | NJ    | 4.4                                  | 26,500           | 24,900                        |
| MO    | 3.2                                  | 300              | 534,900                       | OKd   | 4.3                                  | 4,291,900        | 3,309,100                     |
| ID    | 3.1                                  | 512,100          | 709,700                       | DE    | 4.3                                  | 79,700           | 89,300                        |
| NM    | 2.9                                  | —                | 322,000                       | WY    | 4.2                                  | 120,100          | 156,500                       |
| TXd   | 2.8                                  | 4900             | 3,041,800                     | PA    | 4.2                                  | 144,700          | 102,400                       |
| MTd   | 2.5                                  | 3,459,400        | 2,449,500                     | MD    | 4.0                                  | 210,400          | 116,300                       |
| MN    | 2.0                                  | 1,319,300        | 857,200                       | NC    | 4.0                                  | 753,500          | 688,800                       |
| CA    | 2.0                                  | 175,700          | 385,100                       | OR    | 3.9                                  | 782,200          | 609,300                       |
| NE    | 1.8                                  | 6600             | 675,300                       | IL    | 3.9                                  | 645,800          | 615,600                       |
| NDd   | 1.7                                  | 7,038,200        | 2,798,100                     | AL    | 3.8                                  | 189,400          | 163,200                       |
| NY    | 1.7                                  | 1300             | 40,400                        | TN    | 3.4                                  | 328,200          | 264,400                       |
| SD    | 1.4                                  | 995,500          | 932,900                       | KY    | 3.4                                  | 468,200          | 274,000                       |
| UT    | 0.9                                  | 13,300           | 36,100                        | MS    | 3.4                                  | 346,300          | 223,200                       |
| NV    | 0.8                                  | —                | 2300                          | MO    | 3.2                                  | 690,000          | 581,900                       |
| AZ    | 0.7                                  | 98,100           | 37,400                        | TXd   | 3.2                                  | 2,989,100        | 3,470,800                     |
| NM    | 3.1                                  | 86,400           | 348,300                       | LA    | 3.0                                  | 275,400          | 152,100                       |
| LA    | 2.9                                  | 469,800          | 598,200                       | OH    | 2.9                                  | 300,700          | 140,900                       |
| WA    | 2.6                                  | 1,669,200        | 1,351,000                     | IN    | 2.6                                  | 15,500           | 1900                          |
| FL    | 2.6                                  | 2,168,000        | 2,365,400                     | MT    | 2.5                                  | 2,448,200        | 2,849,900                     |
| AR    | 2.4                                  | 316,100          | 379,100                       | KSd   | 2.3                                  | 9,009,500        | 4,574,500                     |
| CA    | 2.1                                  | 35,700           | 893,100                       | NE    | 2.0                                  | 1,302,700        | 749,500                       |
| MN    | 2.1                                  | 729,200          | 2,805,800                     | ND    | 1.8                                  | 84,800           | 37,400                       |
| NY    | 1.6                                  | —                | —                             |       |                                      |                  |                               |

(Continued)
swaths of rocks that are generally poorly permeable but locally may contain productive aquifers (USGS 2003b). The Other rocks class was removed from consideration because the shallowest sites were localized in the eastern part of the state, opposite the majority of wheat grown in the western half of the state. The next shallowest aquifer was Edwards-Trinity, which did not overlap with any sites in the 85th to 95th percentile concentration range from the screening modeling. So the Blaine aquifer was identified as the shallowest aquifer with a high density of high-concentration wheat sites from which to select the representative scenario for Oklahoma.

There were 67 screening simulations in the 85th to 95th percentile concentration range in the Blaine aquifer. Of these, the simulation corresponding to the largest wheat area (17,723 acres) was selected as the representative scenario. This scenario was characterized as an Aspermont soil series of soil hydrologic group B or C (hydrologic designation depended on the map unit), experiencing weather from Wichita Falls, Texas (SAMSON station 13966). This soil component and weather combination had an areal extent highlighted in yellow in the inset of Figure 7. Note that the spatial resolution of SSURGO data is at the map-unit level, not the component level; therefore, the footprint shown is for all map units with some percentage of this soil component that lie in the SAMSON weather polygon for Wichita Falls.

Applying the same method of site selection used for Oklahoma winter wheat to the remaining scenarios resulted in representative scenarios corresponding to postbreakthrough average concentrations near the 90th percentile (ranging from 88th to 93rd percentiles) for the target states. The average groundwater depths for the principal aquifers associated with the representative scenarios ranged from 3.6 m (CO Denver Basin) to 71.4 m (TX High Plains). These were rounded to the nearest meter and restricted to a maximum of 9 m for the PRZM-GW scenarios. The finalized scenarios were representative of extensive wheat sites. Wheat area for the final scenarios ranged from 13,000 acres (CO winter wheat) to 500,000 acres (ND spring wheat) and was associated with soils and weather conditions found throughout 1 or more counties. The counties corresponding to the representative scenarios are shown in Figure 2. The conditions parameterized by the North Dakota spring wheat scenario were particularly widespread; the chosen vulnerable site occurred in 12 North Dakota counties. This was due to the combination of a weather station’s representative area spanning a large fraction of the state and a common soil component.

The PRZM-GW simulations with the finalized scenarios resulted in similar or lower groundwater concentrations compared to screening modeling. The final postbreakthrough average concentrations ranged from 1.55 µg/L (KS winter wheat) to 4.34 µg/L (CO winter wheat). Breakthrough began as soon as 16 y (CO winter wheat) into the simulation and as late as 89 y (KS winter wheat). The most notable changes from screening results were reductions in the postbreakthrough average concentrations in the Texas and Kansas winter wheat scenarios from 3.25 and 2.36 µg/L to 2.55 and 1.55 µg/L, respectively. These changes were the result of a deeper soil profile that delayed the start of the breakthrough period to the very end of the simulation (82 y for TX and 89 y for KS).

### DISCUSSION

Counties with the soils, weather, and aquifers of the finalized representative vulnerable wheat scenarios are summarized in Table 4 and shown in Figure 2 for comparison to the USEPA standard scenario locations and wheat footprint. The new wheat scenarios add geographic balance to the current set of scenarios by representing environmental conditions in the central and northwestern United States. They also address a deficiency in the diversity of crop classes represented by the standard scenarios, which include only citrus, potato, peanuts, corn, and cotton, and no grain or wheat crops.

Concentrations estimated for risk assessments based on crops and locations not associated with typical use of the pesticide may differ from concentrations based on more representative scenarios. Therefore, it is important to model the actual crop, region, and environment for a given pesticide use to prevent arriving at incorrect exposure conclusions. To

### Table 3. (Continued)

| Spring wheat | Winter wheat |
|--------------|-------------|
| State        | 90th percentile concentration (µg/L)<sup>a</sup> | Harvested acres<sup>b</sup> | Concentration-area integral<sup>c</sup> | State | 90th percentile concentration (µg/L)<sup>a</sup> | Harvested acres<sup>b</sup> | Concentration-area integral<sup>c</sup> |
|--------------|-------------|-----------------|-----------------|-----------------|-------------|-----------------|-----------------|
| SD           | 1.4         | 1,208,300       | 996,400         | UT              | 0.8         | 124,800         | 30,200          |
| UT           | 0.8         | 124,800         | 30,200          | AZ              | 0.7         | —               | 33,000          |
| NV           | 0.6         | —               | 1,700           |

<sup>a</sup> Area-weighted 90th percentile postbreakthrough average concentrations over all screening simulations for each state.

<sup>b</sup> National Agricultural Statistics Service 2012 Census of Agriculture harvested wheat acres (NASS 2014). “—” indicates too few growers in the state to report acreage.

<sup>c</sup> Area-weighted sum of postbreakthrough average groundwater concentrations between 85th and 95th percentile concentrations for the state.

<sup>d</sup> Representative scenarios were developed for these 4 spring wheat and 4 winter wheat states.
Table 4. Summary of representative vulnerable spring and winter wheat scenarios compared to USEPA standard scenarios

| State | Crop      | Soil; hydrologic group | Weather | Percentile (%) | Aquifer | Area (acre) | Local GW depth (m) | GW depth used in PRZM (m) | Pan evaporation factor | Screening PBT avg conc (µg/L) | Final PBT avg conc (µg/L) | Time to breakthrough (d (y)) | Counties                          |
|-------|-----------|------------------------|---------|----------------|---------|-------------|-------------------|----------------------|---------------------|-----------------------------|-----------------------------|--------------------------|----------------------------------|
| OK    | Winter wheat | Aspermont; B or C | Wichita Falls, TX | 88.6 | Blaine | 17723 | 11.8 | 9 | 0.69 | 4.21 | 4.14 | 6369 (17) | Harmon, Greer, Jackson |
| TX    | Winter wheat | Dallam; B | Amarillo, TX | 90.8 | High Plains | 37528 | 71.4 | 9 | 0.685 | 3.25 | 2.55 | 29888 (82) | Dallam |
| KS    | Winter wheat | Colby; B | Goodland, KS | 90.3 | High Plains | 66234 | 27.2 | 9 | 0.69 | 2.36 | 1.55 | 32452 (89) | Cheyenne, Rawlins, Wallace, Logan, Greeley |
| CO    | Winter wheat | Olney; B | Boulder/Denver, CO | 88.4 | Denver Basin | 13444 | 3.6 | 4 | 0.7 | 4.35 | 4.34 | 5776 (16) | Weld |
| ND    | Spring wheat | Zahl; B | Minot, ND | 90.9 | Lower Tertiary | 501217 | 4.9 | 5 | 0.73 | 2.08 | 2.04 | 12728 (35) | Divide, Burke, Williams, Mountrial, Ward, McKenzie, Dunn, Mercer, McLean, McHenry, Renville, Sheridan |
| MT    | Spring wheat | Lohler; B or C | Glasgow, MT | 90.4 | Lower Tertiary | 14245 | 4.9 | 5 | 0.71 | 2.59 | 2.55 | 12654 (35) | Daniels, Roosevelt |
| WA    | Spring wheat | Shano; B | Spokane, WA | 93.0 | Columbia Plateau basaltic-rocks | 133386 | 12.0 | 9 | 0.71 | 4.38 | 4.3 | 12735 (35) | Adams |
| TX    | Spring wheat | Miles; B | Wichita Falls, TX | 92.4 | Seymour | 28967 | 12.6 | 9 | 0.69 | 3 | 2.98 | 9429 (26) | Wilbarger, Hardeman |

PRZM-GW Standard Scenarios

| State | Crop | Soil, hydrologic group | Weather | Percentile (%) | Aquifer | Area (acre) | Local GW depth (m) | GW depth used in PRZM (m) | Pan evaporation factor | Screening PBT avg conc (µg/L) | Final PBT avg conc (µg/L) | Time to breakthrough (d (y)) | Counties |
|-------|------|------------------------|---------|----------------|---------|-------------|-------------------|----------------------|---------------------|-----------------------------|-----------------------------|--------------------------|----------|
| FL    | Citrus | Candler, Tavares, Astatula; A | Tampa, FL | — | — | — | — | — | 3 | 0.78 | 6.62 | 6.49 | 2169 (5.9) | Polk |
|       | Potato | Pomona; A | Jacksonville, FL | — | — | — | — | — | 3 | 0.77 | 0.334 | 0.312 | 3710 (10.2) | Saint Johns |
illustrate this point, PRZM-GW was simulated for the
standard scenarios using the same herbicide chemical
properties and spring and winter wheat application
patterns from the screening modeling. The highest USEPA
PRZM-GW standard scenario concentration (WI corn) was
$2^2$ higher than the highest wheat scenario concentration
(CO winter wheat) and $6^2$ higher than the lowest wheat
scenario concentration (KS winter wheat), as shown in
Table 4. Postbreakthrough average concentrations for all 8
wheat scenarios were lower than 4 of the USEPA 6
standard scenarios (FL citrus, Delmarva sweet corn, NC
cotton, and WI corn). The postbreakthrough average
concentration for Kansas winter wheat was also lower than
the Georgia peanuts standard scenario. The Florida
potato scenario resulted in the lowest concentrations of
all standard and wheat scenarios. Comparing the time for
herbicide to break through to the water table further
highlights the potential for different vulnerability and
exposure conclusions to be made, depending on the
scenarios evaluated. The breakthrough times for the wheat
scenarios, which ranged from 16 to 89 y, were 1.4 to 7.5 x
longer than the standard scenario with the longest
breakthrough time (WI corn, 11.8 y). Long breakthrough
times were common in the nonirrigated central and
western United States, where low annual precipitation
delays the time it takes for pesticides to leach into the
water table.

The 8 new wheat scenarios were developed following
USEPA PRZM-GW exposure assessment guidance for Tier
2 refined modeling because the standard scenarios did
not represent pesticide use on wheat. These vulnerable
wheat scenarios are now available as online Supplemental
Data for inclusion in Tier 1 PRZM-GW exposure modeling.
The new wheat scenarios are appropriate for PRZM-GW
modeling in risk assessments for other chemicals that have
similar mobility and degradation properties as the
herbicide used to identify the representative wheat
scenarios.

Additionally, the systematic approach to scenario identi-
fication could be applied to other pesticides and crops not
addressed by the wheat scenarios or by the USEPA
standard scenarios. The use of python scripting in the
approach facilitates extending the process to additional
pesticide use sites. Python scripts were developed to run
batches of screening simulations simultaneously, thereby
improving processing efficiency, enabling a nationwide
assessment of high-resolution site conditions and ensuring
the reproducibility of results.

Uncertainty

The goal of PRZM-GW modeling was to compare the
relative vulnerability of groundwater concentrations and
identify appropriately vulnerable soil and weather combina-
tions using the conservatively parameterized USEPA
conceptual model; therefore, no formal calibration or
validation of the results was conducted. Parameterized
this way, PRZM-GW has been found to provide upper
bounds on groundwater concentrations (HC and USEPA 2012; OPP 2015), so the results from the screening modeling are conservatively biased high. To achieve groundwater concentrations appropriate for comparison to monitoring data, many of the USEPA model input parameters and assumptions would need to be revised to better represent actual agricultural fields near shallow groundwater wells, for example, using realistic rather than negligible runoff and erosion. The validity of PRZM-GW for exposure modeling and assessments has been addressed by previous publications (including HC and USEPA 2012; Estes et al. 2015), and so it was not necessary to revisit here.

Additional sources of uncertainty in the model results may be introduced by the spatially varying soil and weather input parameters. The SSURGO horizon data typically extended to only the top 1 m of the soil profile, yet PRZM-GW required soil properties to depths of 4 to 9 m. Properties throughout the bottom horizon (>1 m) were biased toward values reported at or near the top of the bottom horizon. Components were excluded from modeling where there were not sufficient data to characterize at least the top 1 m of the soil profile. Even with these omissions, 91% of all soil areas co-occurring with wheat nationwide were modeled. The network of SAMSON weather stations is somewhat coarse, which led to simulating the same weather time series across large areas, especially for less populous states like North Dakota and Montana. Simulating more localized weather would have resulted in smaller areas corresponding to the final scenarios. However, changes in the range of predicted concentrations would be minimal because a wide variety of weather conditions were sampled over time with the 30-y data sets. In addition, long-term average concentrations are not as sensitive to daily fluctuations as much as the overall trend and accumulated moisture.

Uncertainty also exists in the principal aquifer depths, which are important in determining the time to breakthrough. Although aquifer depths were based on the best available daily groundwater data, which were well resolved in time, the wells were geographically sparse, especially in the central and western United States, as seen in Figure 5. Several aquifers had only 1 daily monitoring site associated with the national aquifers, and 2 of the states of interest (MT, KS) had no sites. This necessitated extrapolating the annual average site depths to aquifer-average depths and using aquifer-average data from neighboring states as surrogates. The coarse spatial resolution of the groundwater monitoring sites means that locally shallower areas may have been omitted from the aquifer-average depth calculations. On the other hand, the groundwater monitoring sites included in the aquifer averages were not filtered for proximity to surface waters where some of the shallowest depths were for sites in or near large surface waters. Given these uncertainties, it was
important to evaluate the vulnerability impacts of groundwater depth separately from soil and weather factors by conducting all screening modeling at the constant shallow depth of 4 m. Varying the groundwater depth to 3 m and 5 m (±25%), for the Colorado winter wheat scenario, changed the concentration by less than ±1% and changed the time to breakthrough ±22%. After the soil–weather combinations resulting in high concentrations were identified, groundwater depth considerations were factored into the vulnerability. Even though the groundwater data were limited, they indicated that aquifers in the vulnerable wheat states were generally deeper, on average, than the upper limit of 9 m imposed on the scenarios. Deeper groundwater would generally result in longer times to breakthrough and more simulations with no breakthrough in the 100-y period.

CONCLUSIONS
National screening-level PRZM-GW modeling was conducted for wheat-growing regions with soils characterized at the component level. States with high modeled groundwater concentrations affecting large areas of wheat production were selected for representative scenario development. The combination of these 2 factors in the definition of vulnerable locations was important to establishing not just the conditions leading to high concentrations but also the likelihood of occurrence of impacted areas. Wheat sites corresponding to high postbreakthrough average herbicide concentrations, shallow depth to groundwater, and high herbicide acreage were selected as representative scenarios for each state.

This process resulted in 8 new highly vulnerable PRZM-GW modeling scenarios for wheat crops in regions previously excluded from USEPA standard groundwater scenarios. Furthermore, the concentrations predicted at USEPA standard scenario locations, in the absence of the new wheat scenarios, would not have adequately represented herbicide concentrations in major wheat regions for use in exposure assessments. Groundwater concentrations at the vulnerable wheat sites were lower than most of the standard scenario concentrations, and exposure occurred later in the simulation.

The newly developed wheat scenarios are appropriate and available for use with other chemicals similar to the herbicide modeled here and could be employed in Tier 1 exposure modeling for regulatory groundwater risk assessments. In addition, the methodology outlined by the present work may be applied to systematically identify vulnerable scenarios for additional crops not currently captured by existing regulatory scenarios.

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Data Accessibility—Data are available upon request from the authors. Contact natalia.peranginangin@syngenta.com.

SUPPLEMENTAL DATA
PRZM-GW model scenario input files for the final 8 representative wheat crops and regions are provided as zipped text files.

Table S1. Wheat growth and herbicide application timing
Table S2. Groundwater temperature and minimum evaporation depth by state
Table S3. Summary of additional PRZM-GW input parameters. PRZM-GW = US Environmental Protection Agency Pesticide Root Zone Model for Groundwater.
Table S4. Summary of representative vulnerable spring and winter wheat scenarios compared to USEPA standard scenarios. USEPA = US Environmental Protection Agency.

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