glyphosate, AMPA, and *N*-methylAMPA (MeAMPA), having filtered out interfering signals from unlabeled molecules. MOPS peaks are comparable in size to those of the low concentration metabolites, as seen by comparison of the ^{2}H spectrum of a sample of the mixed Dworkin–Foster/MOPS medium alone (B) with that of the 33-h incubation (C). This background signal led to difficulties in definitively assigning metabolites in the deuterium spectrum, as did uncancelled MOPS peaks in the TRIED spectrum. [^{2}H–^{13}C] INEPT was utilized in an attempt to minimize interactions by combining magnetization transfer from deuterium to carbon.

An 80 mM MOPS solution in D_2O of approximately 15 mg of dideuterated glyphosate (^{13}C–^{15}N–^{13}C-labeled, 75% ^{2}H-enriched at the carboxymethylene protons) was prepared and studied by (A) proton, (B) proton, and (C) [^{2}H–^{13}C] INEPT, Fig 2. MOPS is again the dominant feature of both the proton and carbon spectra. In the [^{2}H–^{13}C] INEPT spectrum, however, only resonances resulting from the carboxymethylene of the glyphosate are detected. The MOPS peaks have been filtered out, leaving only the resonances of the desired compound. [^{2}H–^{13}C] INEPT has a theoretical molar cancellation efficiency of greater than 5×10^5:1 in addition to the increased chemical shift dispersion of carbon. Together, TRIED, [^{2}H]NMR and [^{2}H–^{13}C] INEPT form a powerful arsenal of isotope-edited techniques for the study of glyphosate metabolism in extracts from biological systems.

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Approaches to refining pesticide risk assessments – the spatial estimation of potential leaching risk

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Abstract: A Geographic Information System (GIS) has been combined with a simple leaching model to characterize the factors that influence pesticide leaching, and to identify the spatial distribution of these factors. The results were compared with those of a conventional simulation modeling approach, and a strong correlation was found for 40 selected sites in central and eastern USA.

Keywords: pesticide leaching; geographic information system; production

Addressing the landscape-wide risk of pesticide leaching in areas of chemical-intensive production has been one of the significant recent research topics in agriculture. Although simulation models are commonly used, the spatial variation in pesticide leaching cannot adequately be described on a large scale by such models. Kellogg *et al*[1] and Battaglin and Goolsby[2] developed a US nationwide map of ground-water vulnerability by using a Geographic Information System (GIS) which integrated information on hydrology, major resource areas, federal lands, and county boundaries. A GIS (ESRI Arc/Info, 1996) is a computer analysis and mapping system that was designed for data retrieval, storage, analysis and data presentation. GIS offers a tool for spatial analysis while simulation modeling provides a means for assessment of potential transport through the soil profile at a specific location. The integration of GIS and simulation modeling becomes useful and inevitable in risk assessment at a landscape scale.[3]

This study focused on combining a simple leaching model with GIS to characterize the factors that influence leaching and to identify the spatial distribution of these factors, and then validated the results against simulation models. The study objectives were to investigate and develop GIS tools to examine the environmental fate and exposure arising from use of Zeneca products, to verify GIS relative leaching predictions using Pesticide Root Zone Model[4] (PRMZ2) outputs, and to identify areas with a high risk of leaching of herbicides.

To test the utility of the tools, we selected a potentially mobile herbicide. We applied a GIS map overlay, simple leaching ranking criteria for precipitation and temperature, a soil leaching screening model,[5] statistics, and Kriging geostatistics. Datasets used included STATSGO (NRSC, USDA), cropping agricultural statistics (USDA, 1992) and weather information (Earth Info, Inc.).

The analysis of chemical dissipation and environmental fate indicated the following four principal factors that affect chemical fate: cropping systems, soil-water related properties, precipitation and temperature. By using detailed knowledge of the environment behavior of the herbicide and appropriately weighting and then combining these factors contributing to leaching risk, it was possible to define an overall leaching risk index (OLR). Three of the principal factors were weighted as follows: soil

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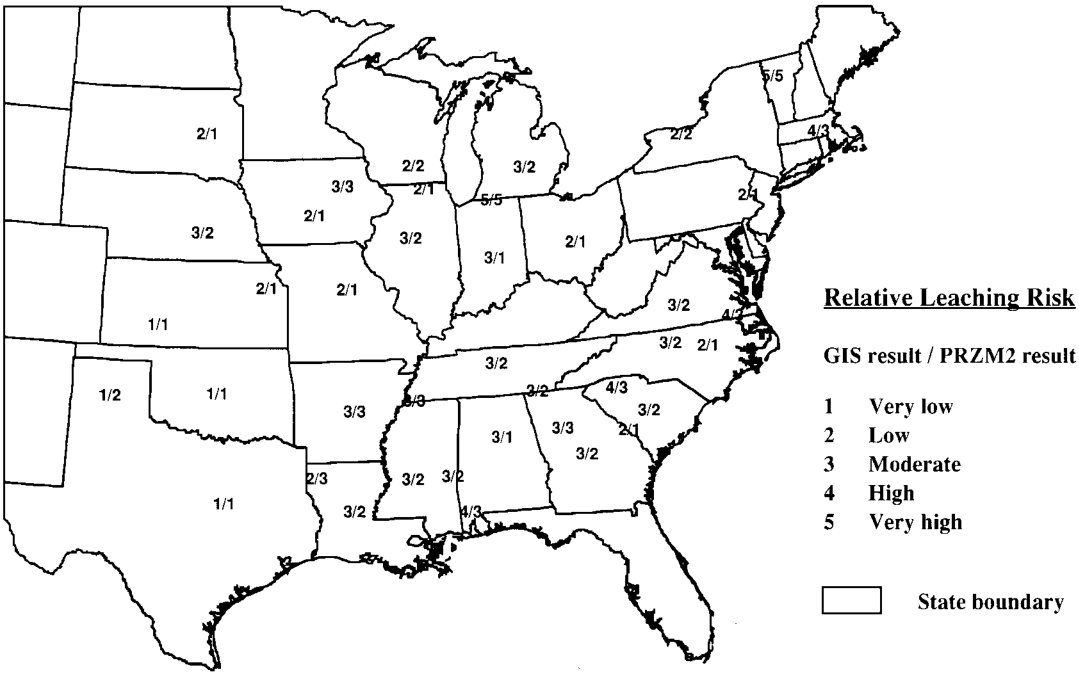

Figure 1. Comparison of results from GIS analysis and the PRZM2 model.

risk 50%, precipitation 33% and temperature 17%. The crop risk index was either 0 (where relevant crops amounted to <5% of the agricultural acres in the county) or 1, i.e.

$$\text{OLR} = \text{f}\{(50\% \text{ Soil}, 33\% \text{ Precipitation}, 17\% \text{ Temperature}) \times \text{Crop index}\}$$

For example, areas with different levels of precipitation were assigned relative leaching risk indices proportional to rainfall levels because potential leaching risk increases with increasing rainfall. The impact of increasing summer temperature was to decrease potential leaching risk index due to increased herbicide degradation.

After integrating cropping patterns, soil properties, precipitation and temperature in the context of the specific environmental behavior of the herbicide, we developed a spatial map illustrating the areas of relative leaching potential. OLR values were allocated by STATSGO map unit area corresponding to those areas where a particular soil association was coincident with a given rainfall, temperature, and cropping pattern.

To compare these results with the conventional simulation modeling approach, the model PRZM2[4] was used to estimate annual mean leachate concentrations at the bottom of the root zone for the herbicide at 40 randomly selected sites across the range of OLR values. The one-in-ten-year worst-case concentrations from PRZM2 were used to rank the sites for comparison with the OLR. Numbers in Fig 1 illustrate examples of the relative leaching in GIS outputs. The different numbers represent the relative leaching intensities.

Analysis of the GIS and model outputs indicated a strong correlation ($r > 0.9$) between mapping and model approaches for the 40 selected sites in the middle and eastern USA. This result increased our confidence that an analysis based on a relatively coarse spatial resolution could be relied upon to give a good relative measure of landscape leaching risk. The approach of using GIS and PRZM2 provides a tool to understand relative chemical leaching potential on a broad spatial scale.

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