Interfacing geographical information systems and pesticide models

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Simulation models offer a complementary role to monitoring pesticides with additional advantages like being cost-effective, linking their transport with use, forecasting of chemical fate before it is used, etc. Pesticide fate modelling coupled with the advantage of GIS technologies for various data-handling, spatial analyses and visualization under variable inputs and spatial scales, is an innovative approach developed during recent years. The use of GIS as a tool for management and analysis of spatial data together with various modelling techniques has many applications in determining pesticide fate in the environment. Applications of GIS, some popular pesticide models with GIS interfaces and their applications have been discussed here.

Keywords: Contamination, GIS, pesticide models, spatial data.

PESTICIDES differ from other chemicals because these are deliberately spread in the environment and are not completely selective for target organisms. These are important inputs in modern agriculture and are also used in public health to control communicable diseases. The intrinsic toxicity of these compounds may represent a risk to human health, environment and non-target organisms. The fate of pesticides and the potential for their movement from the site of application are affected by chemical and physical properties of the pesticide, site characteristics such as soil, geology, vegetation and local weather conditions, and the handling practices of the pesticide user.

Modelling is increasingly being used as a tool for evaluating the transport and fate of pesticides in soil–water systems. An extensive review of pesticide simulation models has been done by Wagenet and Rao[1]. The use of mathematical models simulating pesticide fate is cost- and time-effective, offers the possibility of encompassing the variability in weather conditions through the use of long-term meteorological datasets and also offers extrapolation capabilities to other climates, soil and cropping practices[2–4]. These benefits have led to the development of a large number of models capable of simulating pesticide fate in the environment[5–14]. Some of the models used for assessing pesticide concentration in soil, surface/groundwater and air are: PRZM[15,16], PELMO[17,18], PESTLA/PEARL[14,19,20], and MACRO[10,21]. However, most of these models were developed for studies related to specific problems for limited spatial and temporal scopes. Over time, this research led to the lack of effective basis for supporting formulation of relevant pollution control schemes, policies and regulations.

With the rapid development of Geographic Information System (GIS) as an effective spatial tool, its application in pesticide transport modelling has become a prospective research support. GIS is an automated approach to locational and non-locational data synthesis, which combines a system capable of data capture, storage, retrieval, analysis, manipulation and display[22]. Traditionally, the use of GIS technology has been limited to manipulating geographic databases and producing maps. Recently, however, this rapidly emerging technology has been used extensively for planning water quality protection programmes and in studying environmental degradation processes[23,24].

An important issue in pesticide fate modelling is that all the basic units (water, soil, chemicals and weather) have a spatial distribution and since this distribution considerably affects the processes and dynamics of their interaction, model-based simulations alone are not sufficient. Simulation models have been primarily designed for extensive analysis of large datasets and they can be more effective with the visualization and spatial analysis capabilities that GIS adds to them. Hence the integration of pesticide fate models with GIS interface is emerging as an important tool, which is more accessible and functional. The requirement to link models with comprehensive spatial datasets describing important environmental variables is best achieved within the framework of a GIS[25].

In environmental modelling, several alternatives of GIS applications have been described[26,27]. The spatial characterization of pesticide pollution requires a tool that can effectively manage spatial data. Spatial modelling with GIS is a proven method that is well documented[28–31]. One of the main advantages of GIS is that it can store large amounts of spatial and non-spatial datasets in a common format that can be used for more than one application. Because GIS has the capability of physically referencing data to the earth, different data layers, or themes, can be stored in one database. The collection and development of GIS data layers can sometimes be costly and time-consuming, but once data are stored in a GIS database, they can be used for multiple applications. Data within a GIS database can

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*For correspondence. (e-mail: rmbhagat@hillagric.ernet.in) also be shared among multiple users. These characteristics of GIS make it flexible in current uses and adaptable to future developments in the field of spatial modelling.

Further, the capability to implement models in a GIS environment has spurred a fast increase in the number of models used to predict soil loss, sediment yield, nutrient loss, and pollutant transport in a watershed. Some of these models are AGNPS (Agricultural Nonpoint Source)[32]; SWAT (Soil and Water Assessment Tool)[33], ANSWERS (Aerial Nonpoint Source Watershed Response Simulation)[34] and HSPF (Hydrologic Simulation Program-Fortran)[35]. The integrated use of GIS and prediction models can be considered a powerful means to support decision makers in identifying areas at risk of pesticide contamination.

The integration of models with GIS has a number of advantages such as short running time and quick production of results[36]. Further, interfacing GIS with pesticide fate models is attractive because it permits the simultaneous examination of spatial and temporal phenomena. The present review contains valuable information on some of the recently developed applications of pesticide models with GIS linking, combining or interfacing, i.e. spatial modelling. Linking is defined as merely passing input and output between a GIS and a model; combining is defined as automatic data exchange and GIS tool functions, and integrating is defined as embedding a model in a GIS or vice versa. The main attraction of interfacing models and GIS is to facilitate simultaneous analysis of spatial and temporal variation in processes. Our understanding and interpretation of the simulation results is improved by spatially visualizing the results of models[37]. The advanced spatial analyses further clarify and improve the simulation results[38,39].

Modelling pesticide movement

The release of pesticides into the environment is followed by a series of complex events which transport the pesticide through the air or water, into the ground or even into living organisms following many possible pathways, viz. degradation, transport and accumulation[40]. Pesticides may travel through the atmosphere, soil, surface water, and the organisms that inhabit these media. Several factors such as volatilization, photolysis uptake by plants, or leaching below sampling depth jointly contribute to pesticide losses in the field. The nature of pesticide transport and transformation processes in a soil–plant–air system depends upon the chemical partitioning process[41], which has been interpreted using different models either in a single medium or using multi-compartment approach.

The application of GIS in pesticide fate modelling can be grouped into three categories: (i) existing models that are linked with GIS; (ii) pesticide transport is modelled entirely within GIS, and (iii) GIS is utilized to extract spatial data required for analysis of pesticide pollution. Some of the typical GIS integrated pesticide models and other GIS applications are discussed below.

Models linked to GIS

The hybrid models (GIS <=> Pollutant Model) are dominant systems in modelling pesticide pollution. The term interfacing can be used for the simultaneous use of GIS and modelling tools, since these do not imply a specific level of interaction between them. The terms linking, combining and integrating have been defined for different degrees of interfacing[27,42]. Some of the few most popular pollution and extensively used models that are linked with GIS are reviewed as under:

AGNPS: The AGNPS model was originally developed by United States Department of Agricultural Research Service (USDA ARS)[43]. AGNPS is the single event base and parameter simulation model. The model is used to predict surface run-off volume, peak flow rate, soil loss, sediment, nutrient and pesticide yield in a watershed. It is intended to provide basic information on water quality to be used to classify nonpoint source pollution problems in agricultural watersheds. The new version of AGNPS estimates pesticide movement in soil and run-off. For simulation purposes, the watershed is subdivided into homogeneous land areas (cells) with respect to soil type, land use, and land management. These areas can be of any shape, from square grid cells to hydrologic boundaries. Due to the large amount of input data required, the application[44–46] of AGNPS is limited to watersheds not larger than 200 km^2. However, it has been applied to large basins, by representing the study area by a grid of cells larger than 16 ha. For example, Morse *et al.*[47] applied AGNPS with 100 ha cells to estimate concentrations in a 1645 km^2 watershed.

AGNPS and GIS together have been widely used for modelling water quality processes that included pesticides. A daily mass balance is computed for each pesticide. Annualized AGNPS allows simulations for any number of pesticides, each with its own independent chemical properties. Each pesticide is treated separately, independent equilibration is assumed for each pesticide. Major components of the pesticide model include foliage wash-off, vertical transport in the soil profile, and degradation. Soluble and sediment-adsorbed fractions are calculated for each cell on a daily basis.

Several efforts have been made to integrate GIS with AGNPS to evaluate agricultural nonpoint source pollution. Tim and Jolly[48] developed an integrated GIS and hydrologic/water quality model using ArcInfo GIS and AGNPS, to evaluate agricultural nonpoint source pollution. At least three interfaces between AGNPS and GRASS (Geographical Resources Analysis Support System) have been constructed: (i) at Michigan State University[49], (ii) by Srinivasan and Engel[50], and (iii) by the Soil Conservation Service as a watershed planning tool in the Hydrologic Unit Water Quality Project (HUWQ)[51]. He *et al.*[49] used an integrated AGNPS and GRASS GIS package, GRASS WATERWORKS, to evaluate the impact of agricultural run-off on water quality in the Case River, a sub-watershed of Saginaw Bay. Mitchell *et al.*[52] developed an integrated AGNPS/GIS (GRASS) system to validate the AGNPS for predicting pesticide run-off from small watersheds of mild topography. Srinivasan and Engel[53] developed a spatial decision support system using AGNPS and GRASS GIS to assess agricultural nonpoint source pollution. GRASS is the major public domain GIS that supports a raster data structure, with data conversion from vector data. It performs the basic GIS functions of data input, storage, manipulation, analysis and display[51]. Jankowski and Haddock[54] coupled AGNPS with PC-Arc/Info, a vector-based GIS. The interface was constructed using Arc/Info macro language (SML), Pascal language and batch programming. Another AGNPS-Arc/Info integrated system was constructed by Tim and Jolly[48] to evaluate effectiveness of several alternative management strategies in reducing sediment pollution in a 417-ha watershed located in southern Iowa. AGNPS has also been linked to other GIS programs, such as: ERDAS (Earth Resources Data Analysis System), a grid cell-based system[55]; Geo/SQL, a vector-based GIS[56]; and IDRISI, a raster-based GIS[57].

PRZM: Pesticide Root Zone Model is a one-dimensional non-deterministic compartmental model for the prediction of chemical movement in unsaturated soils by vertical chromatographic leaching. The original PRZM version developed by Carsel *et al.*[15] has been continuously improved. The model is capable of simulating multiple pesticides simultaneously as separate compounds or parent/daughter relationships, i.e. the transformation of a parent compound as well as its daughter species. The model is also capable of estimating probabilities of concentrations or fluxes in or from these various media for the purpose of performing exposure assessments. PRZM is widely used and accepted, and is supported by the EPA Center for Exposure Assessment Modelling. It is accepted for environmental modelling submitted for pesticide registration, both in the US and in Europe.

Burkart *et al.*[58] have used PRZM with GIS to screen for relative susceptibility to pesticide leaching on a regional scale. Auteri *et al.*[59] have created a modified interface of ArcView, adding a new item to the standard menu (e.g. database, soil model, AF/RF model, PRZM-2 model). Lin *et al.*[60] have also developed a Visual PRZM coupled with ArcView to form an extension called ArcPRZM, which provides an efficient way of simulating agricultural chemical fate at various scales. However, it is still in beta version and no applications have been reported as yet.

SWAT: This is an extended version of the SWRB Simulator for Water Resources in Rural Basins) model[33]. Model components include hydrology, weather, sedimentation, soil temperature, crop growth, nutrients, pesticides and agricultural management. It has been linked with GRASS[46,61] and Arc/Info[62]. The SWAT ArcView extension is another graphical user interface for the SWAT[63]. This interface requires the designation of land use, soil, weather, groundwater, water use, management, soil chemistry, pond and stream water quality data as well as the simulation period, to ensure a successful simulation.

The SWAT–GRASS model has been applied for small-scale modelling as well as for continental scale hydrologic modelling. For example, Jacobson *et al.*[64] evaluated the water quality impacts of the diverse crops and management practices in a 4.6 km^2 subwatershed of the Herrings Marsh Run Watershed in the North Carolina Coastal Plains. Srinivasan and Arnold[61] applied the SWAT–GRASS interface and such data as a map of soils (STATSGO), map of land use (USGS LULC) and a Digital Elevation Model (DEM) to estimate the following features for the entire US: average annual rainfall, average annual total water yield, average annual actual evapotranspiration (plant evapotranspiration was calculated as a function of leaf area, root depth, and irrigation), average annual Penman–Montieth potential evapotranspiration, and annual grain yield and biomass production. The US was divided into 78,863 STATSGO polygons for this analysis[65]. SWAT has also an ArcView extension developed[66]. The interface requires designation of land use, soil, weather, groundwater, water use, management, soil chemistry, pond, and stream water quality data, as well as the simulation period, to ensure a successful simulation. Barnett and Fulcher[67] developed another user-friendly and menu-oriented graphic user interface for streamlining modelling processes involving SWAT model and ARC/INFO GIS. New improvements in SWAT allow complete distribution (via a GIS interface) within the model.

HSPF: Al-Abed and Whiteley[35] linked PC-Arc/Info GIS with the HSPF to simulate the effects of changes in land use and in resource management strategies on the irrigation water quality in the Grand River, Ontario, with a drainage area of 6965 km^2. HSPF simulates both watershed hydrology and water quality[68]. The rainfall is distributed into interception loss, surface run-off, interflow and flow into the lower soil zone or groundwater storage. Soil is divided into three moisture zones: an upper soil zone that influences the rapid run-off, a lower soil zone, and a groundwater storage zone. Some of the water from the groundwater storage becomes stream base flow[69].

The water quality component simulates silt, clay and sand sediment transport, including resuspension and settling processes. It can also calculate nutrient and pesticide concentrations. HSPF simulates such transfer and reaction processes as hydrolysis, oxidation, biodegradation, volatilization, sorption, and chemical exchange between benthic deposits and the water column. The program user must supply parameters for each of the modelled processes[69,70].

The model has been successfully used to determine the environmental fate of atrazine in a watershed[4].

GLEAMS: Groundwater Loading Effects of Agricultural Management Systems is a modified version of the model CREAMS (Chemicals Run-off and Erosion from Agricultural Management Systems)[71], that can be used to estimate nonpoint source pollution loadings of nutrient and pesticide from agricultural areas. Later versions of GLEAMS were modified to simulate the generation and degradation of pesticide metabolites[72]. It contains pesticide and nutrient components that allow the simulation of ten pesticides and metabolites at a time. It predicts run-off, percolation and soil and chemical losses at the edge of the field and from the root zone. GLEAMS allows the user to specify the frequency of model output and changes in input over the simulation periods. The model simulates output in two ways; on a daily time step and through long-term simulations of up to 50 years[73]. It is most useful when simulating long-term effects of the interactions between pesticide properties, soil characteristics, management and climate. Previous work has shown that GLEAMS can be used in a cascade format and can be linked with GIS systems. ArcView-GIS user interface has been linked with GLEAMS to support the development of national and regional estimates of pesticide source loading in run-off and sediment from agricultural areas. The user interface facilitates the preparation of input files for several georeferenced GLEAMS simulations and the generation of map and time-series XY graphical simulation outputs[74].

CMLS: The Chemical Movement through Layered Soils is another screening type model that can serve as a management tool and a decision aid for the application of organic chemicals[9]. It can estimate the movement of chemicals in soils and response to downward movement of water. CMLS divides the soil into as many as 20 layers and calculates the fraction of the applied chemical remaining in the entire soil profile and the position of the solute front at different times based on the piston displacement of water. The soil properties affecting chemical movement (bulk density, permanent wilting, field capacity, water contents and organic carbon content) may vary between layers, but are assumed to be uniform within each layer. Two chemical properties (the partition coefficient normalized to soil-organic carbon and degradation half-life) and several climatic and cultural factors known to affect chemical movement (plant root depth, daily precipitation, irrigation and evapotranspiration amounts) are also required by the model. Although this model was written primarily as a management and educational tool, its performance has been compared favourably with observed data and the predictions of several other pesticide fate models in several U.S. locations[75,76]. The CMLS model has also been combined with GIS to predict the threat to groundwater posed by current herbicide applications[77], and several recent studies have examined the impact of data resolution and input data estimation methods on model outcomes[78,79].

LEACHM: The Leaching Estimation and Chemistry Model is a one-dimensional finite difference model designed to simulate the movement of water and solutes through layered and non-layered soil profiles[80]. This is a deterministic, mechanistic, research-oriented model with correspondingly greater input requirements than many simpler models[76]. The model uses: (i) a variable time step based on allowable water content changes in the soil profile; (ii) Darcy's law and the continuity equation to describe transient water flow; and (iii) calculated water contents and fluxes to solve the convection–dispersion equation and describe the movement of solutes which can adsorb, volatilize and degrade. The model also allows depth- and time-dependent root growth, water use (transpiration) and evaporation[80]. LEACHM has been validated and used as a predictive tool at the plot and field scale[80,81], and several attempts have been made to combine this model with GIS databases for regional scale assessments of leaching behaviour[82–84].

TOPMODEL: This is a rainfall–run-off model that bases its distributed predictions on an analysis of catchment topography. TOPMODEL predicts the relative amount and spatial distribution of subsurface, infiltration excess, and saturation excess overland flow based on surface topography and soil properties[85–88]. The model has been validated with rainfall-discharge data[89–92] and several recent studies have examined its applicability to water quality problems[93,94]. Soil erosion network model, a modified version of TOPMODEL, represents the processes related to pesticides and other organic contaminants. The continued popularity of TOPMODEL can be traced to its structural simplicity and parsimonious parameterization[95].

The calculation of topographic index was done manually for a long time[88]. However, with the advent of GIS and terrain analysis techniques, this procedure is now automated. Several recent studies have demonstrated that the spatial pattern and statistical distribution of the topographic index varies with different grid resolutions and estimation procedures[88,96,97].

Other GIS-Simulation model interfaces: Soil, Environmental and Agricultural Management System (SEAMS) is an ArcView interface to the CMLS model that was developed for watersheds in Florida[98]. This tool consists of several modules for evaluating pesticide risks. The SWMM model has a set of tools for ArcView (SWMMTools) to generate input files. Other models with GIS interfaces include ModFlow and WASP[99,100].

Cronshey *et al.*[101] developed an interface between GRASS and a watershed-scale water quality model, SWRRB (Simulator for Water Resources in Rural Basins). SWRRB uses daily time-step for calculations of sediment yield, routing, as well as pesticide and nutrient fate. Basins are subdivided to account for differences in soils, land use, crops, topography and weather[102]. Basins of several hundred square miles can be studied, but the number of sub-basins is limited to only ten.

PIRANHA is a computer-based ecological risk assessment tool. The system includes a GIS-based facility for locating biological resources potentially at risk from pesticides and industrial chemicals, a toxicological inferencing program for species-to-species extrapolation of acute toxicity (TIP), models for predicting ambient chemical exposures in aquatic and agro-ecosystems (PRZM and EXAMS), and bioaccumulation models for aquatic fauna (FGETS). PIRANHA functions under an interactive platform which incorporates soil, crop, pesticide property and meteorological databases. (Register of Ecological Models).

GIS models (models constructed within GIS): Most of the GIS programs are equipped with a macro language that allows the user to write models within application. For example, Arc/Info has powerful macro language, AML (Arc/Info Macro Language). Various GIS functions, viz. data linkage for spatial analysis, proximity analysis, overlay analysis, spatio-temporal analysis and visualization have multifarious application in pesticide science. GIS modelling had been primarily used for assessing the susceptibility to contamination or identification of the hotspots, identifying and tracking pesticide use concentration/flow rate[103] and exposure assessment[104,105] or pesticide leaching[2]. Identification of such areas requires the creation of a 'spatial database', where data are characterized by geographical co-ordinates. GIS can perform prompt analysis, management and representation of these data.

The hydrological parameters, slope/aspect, flow directions, area, etc., the factors that are involved in movement of pesticides, can be calculated within the GIS software. Based on the grid cell system, the DEM technique is used to provide basic input data for pesticide losses in run-off. Flow direction, slope and aspect of grids can be computed from DEM based on terrain analysis and relative hydrological parameter determination methods[106,107]. Many input parameters required by the model are terrain-based and could be obtained directly or indirectly by GIS techniques, such as land slope, aspect, slope shape factor, field slope length and soil texture.

DRASTIC, a pollution potential model implemented within the GIS, developed by Aller *et al.*[108], was used for examining groundwater pollution in Texas by Atkinson[109]. The results of GIS modelling indicated that susceptibility to pesticide contamination was higher throughout Texas. Reddy and Montas[110] developed a Graphical User Interface (GUI) to a Decision Support System (DSS) for nonpoint source pollution control on watershed scales. The system uses GIS functions of ERDAS IMAGINE for data storage and pre-processing.

GIS has been used for hydrologic assessment, i.e. for the analysis of various hydrologic factors for the purpose of assessing risk or susceptibility to pollution. One example of this type of analysis is the use of GIS for evaluating groundwater contamination potential using the DRASTIC ranking technique developed by the US EPA[111]. Other examples of the nonpoint source assessment techniques have also been described[112,113]. This type of spatial modelling is not based upon a rigorous simulation of physical, chemical or biological processes; rather, it uses weighted indexing schemes to quantify the relative influence of various factors in contributing to pollution problems. Bach *et al.*[114] used a GIS-based model to estimate the losses from diffuse sources in surface waters in Germany for 42 pesticides applied to 11 field crops, vineyards and orchards.

GIS as a tool for spatial data extraction

The most basic application of the GIS is spatial data manipulation, data extraction for further analysis, and presentation of results in map-form. Researchers involved in pesticide fate modelling have also used external GIS linkages along with model outputs for data handling and visualization. GIS tools have been utilized as statistical models to support statistical analysis, to determine variation in pollutant concentration[115]. Parameter estimation is probably the most active area in the GIS field when linked to fate modelling, wherein the objective is to determine and quantify parameters that can be used as input to models through manipulation and analysis of various terrain-related datasets. Reported in the literature are numerous examples where information on land slope, channel slope, soil characteristics and land cover was derived from digital raster and vector data layers[116–119]. Use of GIS to automate the parameterization process for models has also been reported[120–122].

Decision support systems

GIS application along with modelling is also a key to the development of DSS. For the assessment of spatial distribution of pesticides, DSS have also been developed by integrating the pesticide fate model outputs and GIS[123–125]. User-friendly DSS which are developed using these important interfaces, offer an easy access to these models. These provide powerful tools with necessary information of an optimized management planning at different spatial scales that offer solutions to many real problems. The development of the GIS DSS – Drainage Run-off Input of Pesticides in Surface Water – based on model algorithms describing the major pathways of pesticide entry into surface waters has been initiated by the German Federal Environmental Agency (Umweltbundesamt, UBA) in 2000. The tool estimates the quantity of pesticide input from nonpoint sources via surface run-off, tile drainage and spraydrift. Furthermore, the predicted environmental concentration of pesticides in surface waters (PECsw) can be retrieved considering the mean daily inputs of substances into various types of river basins characterized by their daily discharge. A GUI was created to provide users of DSS with easy access to the model algorithms for estimating input quantities of pesticides[126].

Potential for new models?

Descriptions of GIS-based modelling applications mentioned here offer little evidence that GIS software and databases have led to the development of new pesticide fate models during the past decade. Also, they have improved the effective application of these models by helping organize model inputs and display model predictions. The increasing availability of colour displays afforded by GIS has accelerated the development and evaluation of analysis methods and led to improvements in existing models as well as the techniques themselves.

Overall, GIS-based modelling experiences during the past ten years reiterate the need to develop new methods for collecting and characterizing the spatial variability of key processes and properties in landscapes, and the importance of modelling error and uncertainty in spatial databases and their effects on model predictions. Geographic information systems and related technologies (GPS receivers, remote sensing platforms, geostatistical techniques, etc.) can help with the collection and interpretation of these data and by doing so, expedite the development and application of new and improved spatial models of key hydrological land surface/subsurface processes in future years.

The development of conceptual frameworks for the simultaneous use of models and GIS for an authentic, interactive environment is a relatively new field. It offers several opportunities to shift from the traditional desktop to remotely accessible GIS applications that allow for an improved collaborative environmental decision-making, by providing for analysis of 'what-if' land use, land management, and pesticide use options.

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