

Software for pest-management science: computer models and databases from the United States Department of Agriculture – Agricultural Research Service^{†‡}

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Abstract: We present an overview of USDA Agricultural Research Service (ARS) computer models and databases related to pest-management science, emphasizing current developments in environmental risk assessment and management simulation models. The ARS has a unique national interdisciplinary team of researchers in surface and sub-surface hydrology, soil and plant science, systems analysis and pesticide science, who have networked to develop empirical and mechanistic computer models describing the behavior of pests, pest responses to controls and the environmental impact of pest-control methods. Historically, much of this work has been in support of production agriculture and in support of the conservation programs of our ‘action agency’ sister, the Natural Resources Conservation Service (formerly the Soil Conservation Service). Because we are a public agency, our software/database products are generally offered without cost, unless they are developed in cooperation with a private-sector cooperator. Because ARS is a basic and applied research organization, with development of new science as our highest priority, these products tend to be offered on an ‘as-is’ basis with limited user support except for cooperating R&D relationship with other scientists. However, rapid changes in the technology for information analysis and communication continually challenge our way of doing business.

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1 INTRODUCTION

Modern simulation and empirical model and database development are a product of the enormous and friendly computer power available to individual scientists today. We build models and databases because we can do so, more and more easily, sitting at gigahertz PCs wired for almost instantaneous global communication and exchange of information. We can easily store, transform, describe and graphically summarize breathtaking quantities of information. This is fortunate because real agricultural and environmental systems are typically complex and must be analyzed using a systems approach.

Within the past two decades computer models of agricultural soil/plant/water systems have evolved

from objects of suspicion among field scientists and regulators to a mainstream technique for pest management and risk assessment of pest-management technology to ecological systems and humans.^{1–5} Models are simply a continuation of the classical scientific goal of expressing observed behavior in mathematical terms, and of doing it precisely enough to make useful predictions. A validated model also serves as an extremely efficient way to communicate scientific knowledge or, to use the more pragmatic phrase, to achieve technology transfer.

The US Department of Agriculture’s Agricultural Research Service (ARS) has a long history of computer analysis applied to agricultural problems. Wischmeier and Smith’s ‘Universal Soil Loss Equation’ or USLE,⁶

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[†] One of a collection of papers on various aspects of agrochemicals research contributed by staff of the Agricultural Research Service of the United States Department of Agriculture, and collected and organized by Drs RD Wauchope, NN Ragsdale and SO Duke

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a regression equation used for erosion prediction, based on thousands of erosion plot experiments, dates back to the 1950s and is perhaps the most-used product ever created by ARS. CREAMS⁷ and its successor GLEAMS⁸ have been important tools for conservation and water quality programs.⁹ For this overview, we will restrict ourselves to current research on computer applications related to pest management and to environmental impacts of pest management, most from the Natural Resources and Sustainable Agricultural Systems National Programs of ARS. Consult the ARS National Programs web page <http://www.nps.ars.usda.gov/> to scan our research program structure.

A listing of models and databases relevant to the interests of workers in pest management is given in

Table 1. For more information on a particular model or database, contact the ARS scientist listed or visit the web page if available. We will discuss a selection of some of the larger ARS multi-disciplinary projects, all of which involve environmental simulations which include pesticide pollution predictions.

2 ENVIRONMENTAL SIMULATION MODELS

2.1 Groundwater Loading Effects of Agricultural Management Systems (GLEAMS)

GLEAMS⁸ is based on CREAMS,⁷ ARS first non-point pollution model, which was designed to predict surface water runoff from fields and resulting non-point pollution by sediment, nutrients and pesticides. GLEAMS can be used to predict surface water runoff

Table 1. Active USDA-Agricultural Research Service model and database projects related to pest management science

Model/database description	Maintenance and support	Contact
Environmental simulation models: field scale		
GLEAMS [†] (Groundwater Loading Effects of Agricultural Management Systems): field-scale model of sediment, nutrient, pesticide leaching and runoff	By ARS research unit (limited)	Version 2.1: Daren Harmel, dharmel@brc.tamus.edu http://arsserv0tam.u.edu/nrsu/glmsfact.htm Version 3.0: http://www.cpes.peachnet.edu/sewrl/Gleams/gleams_y2k_update.htm
RZWQM [†] (Root Zone Water Quality Model): field-scale hydrology and nutrient/pesticide leaching and runoff prediction model (see text)	By ARS research unit	Laj Ahuja: laj.ahuja@ars.usda.gov Great Plains Systems Research, Ft. Collins, CO
HYDRUS [†] : simulating one- and multi-dimensional transport of water, heat and dissolved agricultural contaminants in soils and groundwater	By ARS research unit and the International Ground Water Modeling Center, Golden, CO	Rien van Genuchten: rvang@ussl.ars.usda.gov http://www.ussl.ars.usda.gov/MODELS/HYDR1D1.HTM http://www.ussl.ars.usda.gov/models/hydrus2d.HTM George E Brown Jr Salinity Laboratory, Riverside, CA
Environmental simulation models: watershed scale		
AnnAGNPS [†] (Annualized Agricultural Non-Point Source model): watershed-scale nonpoint pollution model for chemicals, nutrients and sediments	By ARS research Unit	Ron Bingner: rbingner@ars.usda.gov http://www.sedlab.olemiss.edu/AGNPS.html National Sedimentation Lab, Oxford, MS
SWAT [†] (Soil and Water Assessment Tool): models water, sediment, chemical movement in a large watershed	By ARS research Unit EPA supports SWAT as part of BASINS	Jeff Arnold: arnold@brc.tamus.edu http://www.brc.tamus.edu/swat/index.html EPA: http://www.epa.gov/OST/BASINS/
EAHM (Everglades Agro-Hydrology Model): uses WEPP model hydrology and GLEAMS pesticide algorithms to describe south Florida Agricultural nonpoint pollution	In development by ARS Unit	MR Savabi: rsavabi@saa.ars.usda.gov Subtropical Horticultural Research Unit, Miami, FL
Buffer zone models		
REMM [†] Riparian Ecosystem Management Model: simulation of movement and fate of pollutants in streamside soil/water/plant systems	By ARS research unit	Richard Lowrance: LORENZ@tifon.cpes.peachnet.edu http://sacs.cpes.peachnet.edu/remm/ Southeast Watershed Res Lab, Tifton, GA
Decision support models		
GPFARM [†] (Great Plains Framework for Agricultural Resource Management): decision support system for Great Plains farmers	By ARS research unit	Laj Ahuja: laj.ahuja@ars.usda.gov Great Plains Systems Research, Ft Collins, CO
MARIA [†] (Managing Agricultural Resources through Integrated Assessment): decision support system for conservation planning	In design stage	Laj Ahuja: laj.ahuja@ars.usda.gov Great Plains Systems Research, Ft Collins, CO

Table 1. Continued

Model/database description	Maintenance and support	Contact
CQT-STATS: statistics for calculating risk of pest species survivability and reproduction in commercial shipment of stored fruit	By ARS research unit	Peter Follett pfollett@pbarc.ars.usda.gov Pacific Basin Agricultural Research Center, Hilo, HI
MZA (Management Zone Analyst): sub-field management zone delineation for site-specific crop management (precision agriculture)	No day-to-day support anticipated	Newell Kitchen: kitchenn@missouri.edu http://www.fse.missouri.edu/ars/decision_aids.htm ARS Cropping Systems & Water Quality Research, Columbia MO
Stored Grain Advisor(s): stored grain insect protection decision support systems for farm-stored and commercial elevators	By ARS research unit	Paul W Flinn: flinn@gmprc.ksu.edu http://bru.usgmlr.ksu.edu/proj/sga/index.html US Grain Marketing and Production Res Unit, Manhattan, KS
Pest and pathogen biology models		
MARYBLYT™: predicts fire blight infections of apple and pear trees: assists in scheduling bactericide sprays	Not supported	Jay Norelli: jnorelli@afrc.ars.usda.gov Appalachian Fruit Research Station, Kearneysville, WV afrcweb.usda.gov/fireblight/fb8.htm
PMP (USDA Pathogen Modeling Program): empirical foodborne bacterial pathogen population model: estimates growth, survival and inactivation.	By ARS Research Unit	Mike Tamplin: mtamplin@arserrc.gov http://www.arserrc.gov/mfs/PATHOGEN.htm Microbial Food Safety Research, Wyndmoor PA
SWFSIM (Screwworm Fly Simulation Model): computer model that simulates the influence of weather on growth of the screwworm in a wide geographical range.	By ARS research unit	Dan Haile:HAILED@tivolli.si.edu Screwworm Research Unit, Panama City, Panama http://www.screwworm.ars.usda.gov/
Weedcast: site-specific prediction of weed seedling emergence and growth for 17 weed species	By ARS Research Unit	David Archer: Archer@morris.ars.usda.gov North Central Soil Conservation Research Lab, Morris, MN http://www.morris.ars.usda.gov/morris/products/weedcast/weed2.htm
Spray drift models		
Aerial Spray nozzle atomization models: spreadsheets estimate spray droplet parameters for a given set of application conditions. Used by applicators to comply with droplet spectrum requirements ^{53,54}	By ARS research Unit, coop. With National Ag Aviation Association and Spray Drift Task Force	Ivan Kirk: i-kirk@tamu.edu http://apmru.usda.gov/downloads/downloads.htm Areawide Pest Management Res Unit, College Station, TX
Drift Model: spraydrift and evaporation, droplet temperature changes and droplet impact energy of droplets from irrigation sprinklers and spray heads	By ARS research unit	Dennis Kincaid: Kincaid@nwisrl.ars.usda.gov Northwest Irrigation and Soils Research, Kimberly, ID
Databases		
ARS-PPD (ARS Pesticide Properties Database): critical compilation of environmental parameters for pesticides	Not supported; most newer (<5 years) compounds missing; update in progress	Don Wauchope: don@tifon.usda.gov http://wizard.arsusda.gov/acsl/ppdb.html Southeast Watershed Research Laboratory, Tifton, GA
MedHost: bibliographic database of hosts of Mediterranean fruit fly	By ARS research unit	Grant McQuate gmcquate@pbarc.ars.usda.gov Pacific Basin Agricultural Research Center, Hilo, HI
Plant Disease Databases: rust, karnal bunt, fusarium — bibliography, variety susceptibility, resistance genes, index of fungi, annual surveys	By ARS research unit	Mark Hughes: markh@umn.edu Cereal Disease Laboratory, St. Paul, MN
Modeling support		
OMS† (Object Modeling System): a framework for archiving and configuring modular simulation models	In development	Laj Ahuja: laj.ahuja@ars.usda.gov Great Plains Systems Research, Ft Collins, CO
StormGen: generates synthetic storm-occurrence, depth, duration and within-storm intensity data with seasonal (monthly) dependence	In development	Jim Bonta: bonta@coshocton.ars.usda.gov North Appalachian Experimental Watershed Research, Coshocton, OH

† See text for a more detailed description of model.

from fields, infiltration through the root-zone, and resulting non-point pollution by sediment, nutrients and pesticides both in surface and subsurface flow. GLEAMS added a 'tipping bucket' (layer draining) leaching model and an improved foliar washoff model to CREAMS' algorithms for pesticide runoff and first-order degradation in crop foliage and soil. These algorithms have since been incorporated in most of the ARS environmental models, including SWAT, the Everglades Hydroecosystem version of WEPP, AnnAGNPS and EPIC (see below). GLEAMS is supported by ARS to a limited extent (see Table 1). It has a large user base world-wide and has been applied to several significant national non-point pollution assessment (pesticides, sediment, nutrients) projects.^{9–11} A recently updated version of the model (version 3.0), which is available on the web, but not supported by ARS, includes a turf harvesting scenario, ability to simulate many pesticides, two-phase pesticide degradation, and metabolite tracking.

2.2 The Root Zone Water Quality Model (RZWQM)

Development of RZWQM started at the height of agricultural groundwater pollution concerns. The software was initially designed to function as a more theoretical 'physical' field-scale hydrologic model for leaching and to simulate the effects of agricultural management practices on water quality. However, RZWQM has evolved into a comprehensive one-dimensional field process model for tracking the dynamics of water, pesticides, metabolites and nutrients in a climate/soil/crop system. The model utilizes time steps from minutes to days depending on the process to be described, and may be used to estimate long-term (decades) effects.^{12,13} Applications of the model to a variety of pesticide problems is being reviewed and presented in a series of papers for this Journal.^{14–19} RZWQM is quite complex, but a full Windows™-based user interface has greatly improved its friendliness over the original version. The pesticide model is also reasonably balanced in sophistication in comparison with the rest of the model.

RZWQM currently does not have phosphate and erosion components, but these are under construction. The model may be downloaded from the Web and is currently supported by the developers. A small cadre of researchers is exploring its application to pesticides and testing RZWQM's features against field data, including pesticide soil residue 'aging', soil sorption of weak acid–base pesticides, variable degradation rates in time and depth, volatilization from the soil surface, and controlled-release formulations. It is currently being 'modularized' as a test case for the Object Modeling System modeling environment discussed below.

2.3 The HYDRUS subsurface flow/transport models

HYDRUS-1D²⁰ and HYDRUS-2D²¹ are Windows-based modular modeling environments for addressing

one- and two-dimensional sub-surface flow and contaminant transport problems. The codes have been applied to a variety of pesticide and other contaminant transport problems.^{22–25} The HYDRUS codes use the Richards equation for variably saturated flow and Fickian-based convection–dispersion equations for both heat and solute transport. The solute transport equations include provisions for non-linear sorption, one-site and two-site non-equilibrium transport, physical non-equilibrium and degradate formation and transport. Optimization modules allow estimation of soil hydraulic and solute transport and reaction/degradation parameters from experimental data. A hierarchical set of pedotransfer functions based on a combined bootstrap–neural network procedure predict water retention parameters and saturated and unsaturated hydraulic conductivity, as well as their probability distributions, from soil texture and related data.²⁶ The HYDRUS models are supported by interactive graphics-based interfaces for data pre-processing, generation of structured finite element grids, and graphical interpretation of the results (including animation). The two-dimensional package includes an option of a mesh generator for unstructured finite element grids.

Agricultural applications include pesticide leaching and volatilization, irrigation and drainage design, salinization of irrigated lands, transport of toxic trace elements, non-point source pollution, virus and bacteria transport, and analyses of riparian systems. Future plans²² are to include (a) preferential flow using a range of dual-porosity and dual-permeability flow modules, (b) the fate and transport of colloids, bacteria and pharmaceuticals, (c) colloid-facilitated transport (d) improved geochemistry to account for the transport of organic contaminants, toxic trace elements, or mixtures thereof, (e) surface runoff and sediment transport, (f) constructed wetlands, (g) improved pesticide chemistry, including soil fumigants, and (i) a three-dimensional version.

2.4 Annualized Agricultural Non-Point Source model (AnnAGNPS)

AnnAGNPS is a continuous-simulation (in time) version of the single-rainfall-event AGNPS model.^{27,28} AnnAGNPS is designed to analyze the impact of non-point source pollutants from mixed-land-use (but predominately agricultural) watersheds on the aquatic environment. It consists of a suite of integrated models developed in cooperation with the Natural Resources Conservation Service (NRCS). The modules in addition to AGNPS include: (1) the Conservational Channel Evolution and Pollutant Transport System (CONCEPTS),²⁹ a set of stream network, corridor and water quality computer models designed to predict the effects of bank erosion, bed aggradation and degradation, burial and re-entrainment of contaminants, and streamside riparian vegetation on channel morphology and pollutant loadings; (2) the Stream Network

TEMPerature model (SNTEMP),³⁰ a watershed-scale, stream network, water temperature computer model to predict daily average, minimum and maximum water temperatures; (3) the Sediment Intrusion & Dissolved Oxygen (SIDO) model,³¹ a set of salmonid life-cycle models designed specifically to quantify the impact of pollutant loadings on their spawning and rearing habitats, as well as to include other important life-threatening obstacles; and (4) an economic model that determines the net economic value of Pacific Northwest salmonids restored to either the commercial or recreational catch.

There are a number of additional modules that support the user in developing the needed AnnAGNPS databases. These include: (1) the TOPographic PArAmeterization program³² (TOPAZ), to generate cell and stream network information from a watershed digital elevation model (DEM); (2) the AGricultural watershed FLOWnet generation program (AGFLOW)^{33,34} to format TOPAZ output for AnnAGNPS; (3) the Generation of weather Elements for Multiple applications (GEM) program³⁵ to generate the climate information for AnnAGNPS. Additional programs format and exchange data and provide a graphical user interface including GIS I/O.

2.5 Soil and Water Assessment Tool (SWAT)

SWAT^{36–38} is designed to simulate watershed processes (including watersheds so large that they require longer than one day to respond to storms) and the impact of land and water management on water quality. The model operates on a daily time-step and allows a basin to be subdivided into grid cells or natural sub-watersheds. Model sub-basin components include hydrology, weather, sedimentation, soil temperature, crop growth, nutrients, pesticides and agricultural management. The primary considerations in model development were to stress (1) land management, (2) water quality loadings, (3) flexibility in basin discretization, and (4) continuous time simulation. The model integrates hydrology, soil erosion, plant growth and nutrient cycling with off-site processes such as channel erosion/deposition, pond and reservoir processes, groundwater flow and climate variability. Numerous user interfaces, including geographic information systems (GIS) and web-based tools, have been developed. The model has been validated against measured stream flow and water quality parameters across the USA and in numerous foreign countries.

SWAT has been applied extensively for policy planning and in developing best management practice alternatives. Major projects include: (1) Hydrologic Model of the United States (HUMUS),³⁹ a project between ARS, NRCS and Texas A&M University to simulate stream flow and quality of all major US river basins; (2) integration of SWAT into the US Environmental Protection Agency's BASINS interface and use of SWAT by several EPA programs; (3) providing non-point source pollution estimates along US coastlines for the National Oceanic

and Atmospheric Administration National Coastal Pollutant Discharge Inventory.

The equations used to model the movement of pesticide in the land phase of the hydrologic cycle were adopted from GLEAMS. While an unlimited number of pesticides may be applied to individual sub-watersheds, only one pesticide may be routed through the channel network of the watershed due to the complexity of the processes simulated. The total pesticide load in the channel is partitioned into dissolved and sediment-attached components. While the dissolved pesticide is transported with water, pesticide attached to sediment is affected by sediment transport and deposition processes. The major in-stream processes simulated by the model are settling, burial, resuspension, volatilization, diffusion and transformation.

2.6 Riparian Ecosystem Management Model (REMM)

Riparian buffer systems—streamside areas with natural or planted vegetation that can act as sinks and degradation zones for non-point pollutants, keeping them out of the adjacent water bodies—are a critical agricultural pollution research area in the USA.⁴⁰ REMM⁴¹ is designed to analyze the capabilities of variations of a three-zone buffer design⁴² consisting of (1) an herbaceous filter strip adjacent to the delivering agricultural or other area; (2) a managed (harvested) forest, and (3) a permanent, undisturbed forest adjacent to the water body. Thus, a detailed description of plant species types and their growth and effects on the hydrology and nutrient cycling is required, based on the vegetation used in the three zones. REMM simulates the fate and behavior of nutrients and sediment delivered to such buffers by runoff and lateral sub-surface water flow from upslope agricultural or forest areas. A daily time-step hydrologic model tracks soil water movement in two dimensions (downslope runoff and sub-surface flow in a layered system and leaching between layers) as affected by precipitation, plant interception and evapotranspiration. Channel and overland erosion and deposition are calculated as well as enrichment of fines compared to the parent soil and/or incoming sediment. Carbon, nitrogen and phosphorus pools and processes are modeled in some detail, based on a variety of previous models especially CENTURY, NLEAP and EPIC.^{43–45}

Currently REMM does not have pesticide process descriptions, but building this is a current project of the ARS Laboratory at Tifton.

2.7 Great Plains Framework for Agricultural Resource Management (GPFARM)

'Sustainability' is a complex concept involving management and economic decisions that are impacted by many interrelated variables. GPFARM⁴⁶ is a 'decision support system' which integrates some aspects of artificial intelligence (rule-based systems)⁴⁷ with databases and environmental simulation models, all

put together using object-oriented programming.⁴⁸ The project is a joint effort between ARS and Colorado State University, and recognizes that the development of sustainable farming practices requires a long-term strategic whole-farm systems analysis. GPFARM supports decision-making for a combined crop/livestock operation and attempts to optimize water, nitrogen and pesticide uses, while protecting natural resources. Currently the system is operational, and databases and parameter values have been developed and tested with cooperating Eastern Colorado dryland farm/ranch operations.

2.8 MARIA: Managing Agricultural Resources through Integrated Assessment

Resource conservation planning software used by local conservation agency personnel is primitive compared to current science and information technology, and recent developments in agricultural system models, decision support software, and computer technologies have the potential to provide much-improved tools.⁴⁹ However, use of most complex models still requires significant user expertise. The objective of the MARIA project is to develop a research-information database as a decision support system to help NRCS personnel help producers make timely and more accurate decisions for water quality management. The product will bridge the gap between current science/technology and NRCS water quality conservation planning, so as to address agricultural impacts on water quality. The effects of management from the ARS MSEA projects⁵⁰ and other experimental sites will initially be quantified and evaluated with the Root Zone Water Quality Model (RZWQM) or its hybrid with components from other models. The calibrated/validated models will then be used to extend the database for other soils, climates and potential BMPs in the Midwest. An expert panel from NRCS and ARS will define the range of potential BMPs for model simulation and evaluate simulation results afterwards. An economic package, Procots, will be used to determine economic impacts of simulation results. The information database will be distributed to NRCS personnel through the Internet, based on site-specific soil/weather/management practices. Decision variables for conservation planning and water quality protection in the database will include crop yield and net return, nutrient, pesticides and soil erosion. Uncertainty of simulation results for each endpoint will be provided to help users understand the impact of natural variability and to assess risks of alternatives. The information and decision support system will be developed for a part of Iowa, tested and modified. In a second five-year cycle of the project, the information database will be expanded to include environmental quality concerns besides water quality (eg soil and air quality) and extended to other states (eg in the Great Plains and Southwest).

3 LINKING A LIBRARY OF MODELS: THE OBJECT MODELING SYSTEM OMS

Object-based modeling makes use of the modular architecture of modern software and the power of the graphics interface to provide the user with a visual way to construct collections of interacting pieces of software. The concept has enormous potential to provide archival storage of simulation algorithms which may be integrated to describe complex systems. Accessing a library of tested and validated modules avoids rewriting the code for an equation—or trying to understand someone else's code. OMS is being developed in a collaboration between ARS, NRCS and the US Geological Survey, and is one of several ongoing US Government Agency attempts to harness this concept. A foundation for the OMS project was provided by the work of Leavesley *et al.*^{51,52}

The objectives of the OMS project are to: (1) identify modeling library parts (modules or components) and glean them from existing non-modular simulation models; (2) formalize the linkages between these components to support model building; (3) develop generic software tools to support models and modeling; and finally (4) develop the framework which supports these objectives. The following functional components will be part of the framework:

- 1 A module-building component that will facilitate the integration of existing (legacy) code into the framework. This adaptation support will simplify the technical procedure for module implementation.
- 2 A module repository that will contain modules that can be readily utilized to assemble a working model. Types of modules included in the library are: science-, control-, utility-, assessment- and system-modules.
- 3 A model builder that will assemble modules from the module library into executable models and verify data connectivity and compatibility in scale and comprehensiveness.
- 4 A dictionary framework that will manage extended modeling data type information and provide extended semantics checking for module connectivity verification.
- 5 An extensible user interface that will facilitate an appropriate user interaction for general model development and application. It will be supported by a number of contributing software packages for database management, visualization and model deployment.

For scientists, this means that their specific code can achieve a measure of immortality, because their code becomes reusable as part of other systems, but retains its identity (and attribution). This solves many intransigent problems associated with the interface between research scientists and their agencies' support of their models.

OMS as a framework is operational, and several models (including RZWQM), have been or are being 'modularized' for testing within the framework.

Importantly, the system and its library will (must) be developed in a completely 'open' development environment using the internet: the library will be the product of a global community of scientists.

4 CONCLUSION

We have focussed mostly on environmental, hydrologic, soil- and water-models because these tend to be our agency's emphasis in the systems analysis area. Table 1 lists other software products related to pest management, and these powerful tools are being applied by ARS researchers in many other areas of agriculture, such as land use planning and GIS, crop productivity and climate change. These are extraordinary times for those fortunate enough to have the opportunity to apply the almost unbelievable power of computer technology to one of the most difficult and critical problems facing mankind: the sustainable production of a safe and adequate food supply. Computers and modeling systems will not solve the problem by themselves, but they will certainly be an essential part of the solution.

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