Update

FALL 2002

Stone Environmental News on FIFRA and Environmental Fate Issues

Inside:

The quality and availability of orthophotos has improved such that they now can be used to precisely define small areas where chemicals will be applied, as shown above. For a current pesticide runoff study, Stone used an orthophoto and ArcGIS software to digitize the pesticide application area within a small suburban catchment. Impervious surfaces (rooftops, roadways, sidewalks, and tennis courts), pools, and environmentally sensitive areas (buffers around storm drains, ponds, and children's playgrounds) were excluded. These features are surprisingly easy to see on the high-resolution photo.

Literature Review: Corn Herbicide Loading Studies

As part of a recent watershed characterization study, Stone Environmental conducted a literature review of the factors that affect the transport of corn herbicides in surface waters. Stone found that streamflow and a variety of watershed characteristics were the major influences on herbicide concentrations and loads in rivers.

Streamflow

In many of the studies reviewed, streamflow was a major factor in the mass export of an herbicide from a particular watershed. For instance, in a study in the Chesapeake Bay watershed, streamflow yields (flow unitized by drainage basin area) were directly related to the yields (lbs/mi^2) of the following herbicides: alachlor, atrazine, cyanazine, and simazine (Hainly and Kahn, 1996). Several studies showed that most of the annual herbicide loadings and/or highest herbicide/pesticide concentrations occurred within the first few storm events following application (Crawford, 2001; Fenelon and Moore, 1998; Goolsby and Battaglin, 1995; Louchart et al., 2001; Pope, 1995; Richards, 1998; Richards et al., 1996; Thurman et al., 1991).

A large-volume runoff event long after application time also resulted in large herbicide losses. In the Mississippi River, a flood event in 1993 from mid-June through early

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Are There Simple Steps We Can Take Now?

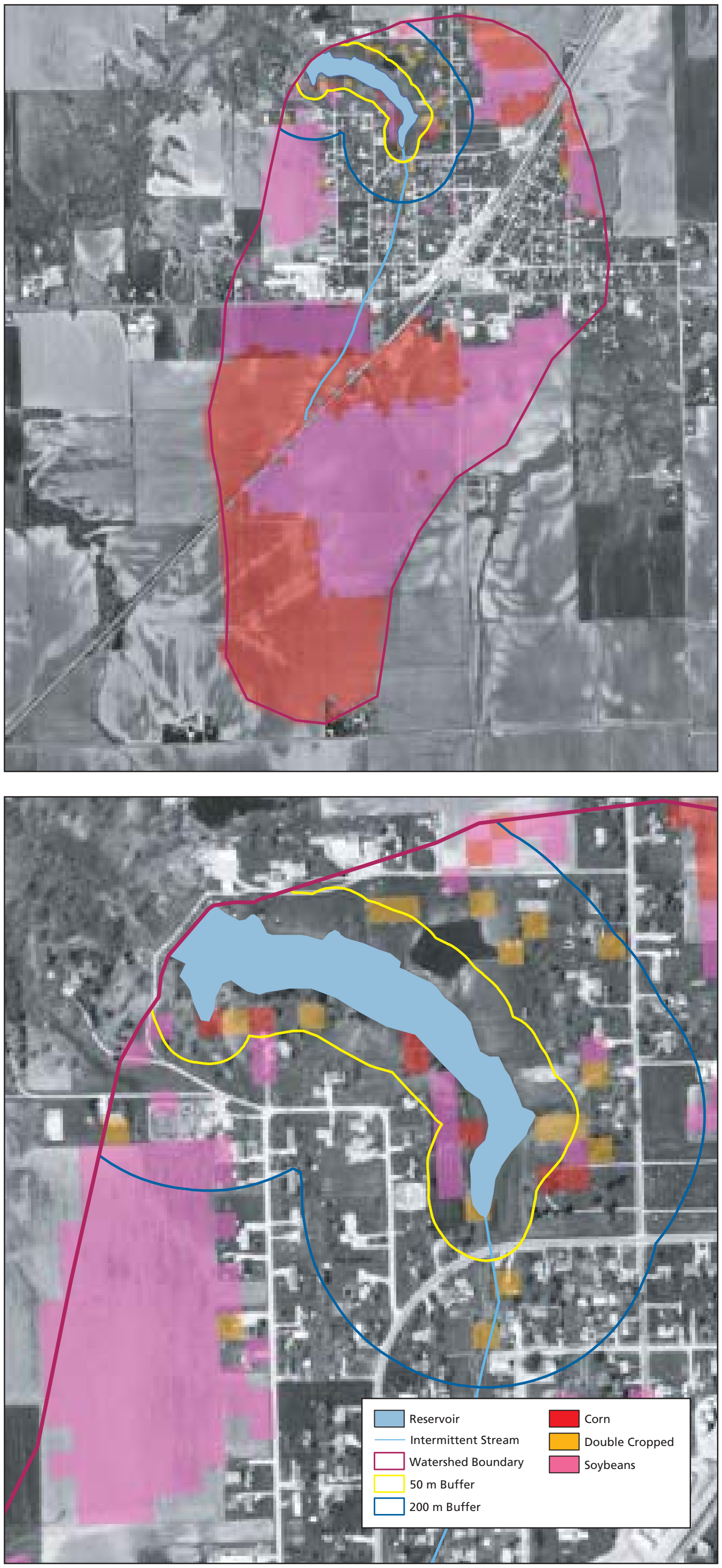
Developing Confidence in Exposure Model Output and Scenarios

A guest editorial by Paul Hendley, Syngenta Crop Protection, Inc.

I was fortunate to be asked to present a talk on *Validation of Exposure Model Predictions for Regulatory Purposes* at the recent 2002 IUPAC meeting, and as I thought about what needed to be said, several interesting perspectives on modeling (and modelers) became apparent. The complete talk will be published in the IUPAC proceedings in due course, but, in the meantime, I am keen to discuss two key issues related to model characterization and scenario development that may merit debate within the US modeling community. I would be very interested in any feedback on these thoughts.

Modeling Under Pressure

My first realization was that the exposure modeling "scene" has changed over the last 10 years. In the past there was a small pool of international experts who all generally understood the strengths and weaknesses of available modeling tools and who typically used the model output to help understand relatively complex pesticide regulatory issues. However, while modeling experts still play an important role today, the typical model user is likely to be less experienced and under more pressure to develop "answers" to deadlines in order to address standard regulatory endpoints for the majority of registration submissions. It is also quite likely that many of these users have diverse backgrounds in ecology and environmental science and do not have the depth of understanding of the processes underlying exposure prediction that experts might expect. If (when!) predicted exposures cause an exceedance of a regulatory level of concern, industry modelers today are expected to perform more sophisticated exposure modeling to refine the risk assessment—often having to use different approaches and models to satisfy different national registration bodies—but almost always under time pressure. On the regulatory side of the fence, the modeling community has also expanded to include users as well as experts who are asked to conduct or review modeling—again under great time pressure to generate data to support decision-making.



The Shipman, Illinois, reservoir was the basis for EPA's Index Reservoir scenario and was parameterized conservatively as a first-tier scenario. However, detailed evaluation of actual crop areas and the reservoir margins that might contribute to drift entry shows that the first-tier parameters greatly exaggerate the true potential for exposure.

General Lack of Confidence

Another significant change is that today, model output is more frequently being used to help resolve risk assessment issues that have environmental, political, and socioeconomic implications. This leads to frequent criticism of the exposure estimates by the "losers" of decisions. Depending upon the circumstances, the critics may be regulators concerned that lenient decisions might be due to industry manipulation of model parameters, industry scientists concerned about overly conservative scenarios, or academics and NGOs perturbed by apparently high levels of uncertainty in the evaluations. As a result of this often strident criticism alongside the long-standing concerns about the "significance and accuracy" of model output, certain regulators and sections of the public continue to have low confidence in modeling relative to field measurements.

Hence, I came to the conclusion that both the modeling community and the uses to which models are put have changed. Therefore, we have a duty and an opportunity to rethink how best to ensure that model output is well understood, transparent, and consistent to build confidence in exposure model estimates among the public and regulators.

Simple Steps to Help Build Confidence Now

Although EPA and industry have been working together to improve many aspects of modeling over the last 10 years, several simple steps could be taken now to improve confidence in regulatory exposure model use.

First, for *every* model used for regulatory purposes, modelers should (1) document the conceptual model underlying the code; (2)

list all inherent assumptions *and* their typical implications; (3) provide clear guidance for input parameter selection and reporting; (4) agree on and list known strengths, weaknesses, and pitfalls of the model in a digestible format; (5) list formal and informal evidence of "suitability for purpose"; (6) document all published information on sensitivity to input parameters; (7) ensure that effective version control, documentation, and "bug reporting" systems exist; and (8) provide a system for maintaining, updating, and revising this information package as the science and/or model code develops.

Second, modelers should agree on a *consistent* international minimum format for reporting model validation and sensitivity studies. This would include a standard suite of test chemicals for sensitivity studies, some of which ideally should be frequently monitored for in groundwater or surface water. It should also include agronomic sensitivities, e.g., the effect of application date on runoff for a given multi-year weather data set. The international format should also incorporate a tiered approach to model calibration/validation, such as (1) understand the quality of hydrology predictions; (2) understand the quality of conserved parameter (e.g., sediment, bromide) predictions; and (3) demonstrate the quality of prediction of daily mass of available chemical. Only then is calibration/validation of predictions of chemical movement in space/distance and time worthwhile.

Third, modelers should refine and agree upon "weight of evidence" approaches for ground-truthing model predictions when rigorous validation is not possible. This can be done by combining information from multiple sources/locations and making existing validation data sets publicly available, including discussion of the strengths and weaknesses of field studies.

Fourth, modelers should use a "moditoring" approach—using monitoring and modeling together in the field.

Fifth, modelers should revise and agree upon a *consistent* "Good Model Practice and Reporting" guidance that requires (1) supplying a formal problem formulation for each model report; (2) documenting all assumptions involved in exposure assessment and their impact on the risk assessment; and (3) identifying any discrepancies between the conceptual model describing transport processes associated with the chemical/use pattern and the characteristics of the selected model.

Scenarios—Quantifying "Reasonable"

The second theme that struck me as I prepared for the presentation was how unproductive the debate has been about the "reasonable worst-case scenario" and how "unreasonable" certain regulatory modeling requirements are. My conclusion is that the industry has behaved somewhat unfairly in criticizing the over-conservatism of scenarios, since regulators traditionally had few alternatives to making rather arbitrary assumptions for early-tier assessments, and additionally, for some types of modeling, higher-tier options were available to refine exposure. However, tools are available today to allow us to select and rank scenarios on the basis of their geographical, ecological, and environmental significance, and therefore I again recommend that we reexamine our processes for understanding and specifying exposure model scenarios.

First, I would argue that there is *nothing wrong* with simplifying assumptions associated with input parameter selection or a scenario *provided that* the assumptions are documented in the report and impacts are understood. For example, EPA Environmental Fate and Effects Division (EFED) reviewers apply a hotly debated "3X safety factor" assumption when only a single aerobic soil degradation input value is available. Simple sensitivity analysis can examine the response of the risk or exposure assessments to this assumption; if they are insensitive, no particular concerns should be generated. However, if this conservative assumption does significantly impact the exposure estimate, then it is reasonable to generate additional degradation data or accept regulatory decisions based on the conservative value.

Similarly, I would argue that (almost) any exposure modeling scenario should be considered to be valid *provided that* the underlying implications and regulatory purposes are understood. I am convinced that there is a lot of room for improvement in scenario development and documentation because to understand the implications of a scenario, it is necessary to understand its regulatory relevance (e.g., tier level and endpoint), its context (e.g., region and crop), and its rank (e.g., this represents a 90th percentile sorghum site in Kansas when erosion potential is ranked). To date, we have largely failed to refine scenarios as exposure refinement progresses; clearly, a protective first-tier model should be conservative, but higher tiers require additional detail.

Shipman, Illinois, Index Reservoir Example

An example of scenario assumption implications for different tiers is given in the figure. EPA defined the Index Reservoir scenario very precisely in terms of watershed, reservoir, and stream dimensions as well as drift entry potential based on the Shipman, IL, watershed; the specification was exemplary for a protective first-tier scenario. However, more detailed examination of recent NASS remote sensing data for Shipman shows that, in reality, the PCA value for corn is 30 percent rather than 46 percent, even assuming 100 percent market share, while, as the diagram shows, there are only minimal amounts of corn within the 50 m or 200 m buffers around the reservoir such that the standard Index Reservoir drift entry assumption (16.8 percent) is inappropriate. This shows why it is important to re-parameterize scenarios as one moves to more refined exposure estimates.

It is interesting that the uncertainty and variability associated with chemical behavior, soils, and weather station selection on model outputs are increasingly being discussed in the US regulatory community despite the fact that a simple analysis suggests that the "basic" assumptions underlying model scenarios often have much greater impacts on exposure estimates. Indeed, it seems likely that these basic assumptions may be a major reason (along with scale factors) that modeled estimates of drinking water concentrations typically exaggerate measured values from monitoring programs.

Thus I believe we urgently need to decide when/whether/how to rank all regulatory scenarios nationally and/or regionally in terms of:

- A desired parameter (e.g., erosion or leaching potential based on local weather).
- Percent Crop Area factor for watershed.
- Landform (e.g., drainage area to water body volume).
- Crop-specific environmental variables (e.g., using only soils and slopes associated with a particular crop).
- Water body environmental and ecological relevance (e.g., pond, stream, ditch).
- Percent of crop in watershed treated with chemical of interest.
- Whether water overflow occurs from static water bodies.
- The extent of proximity between crops and the water body where spray drift is an issue.
- The impacts of mitigating land covers between crops and water for reducing drift or runoff.

The first four points should probably be included even for second-tier scenarios, and the others may be used as appropriate in further exposure refinements. The excellent availability of classified remote sensing and GIS data in the US means we already have the tools to perform these rankings. In combination with the detailed scenario documentation currently being instituted by EFED, a joint industry–EPA effort to develop the science for ranking scenarios would go a long way toward building regulatory confidence in the significance of model output.

If we addressed these two issues now, modeled exposure estimates would still be conservative but would more closely approach monitoring results and therefore would lay the foundations for rebuilding confidence that they are suitable tools for regulatory decision-making.

For discussion, please contact Paul Hendley at Syngenta Crop Protection Inc. via (336) 632-6112 or paul.hendley@syngenta.com.

Susan Alexander

Kim Watson

Tammara Estes

Susan Alexander, FIFRA group leader, and **Kim Watson**, QA manager, exhibited at the 2002 NAICC Annual Meeting in Albuquerque, NM, in January. Ms. Watson also attended the two-day training on *Good Laboratory Practices for the Field* sponsored by Syngenta Crop Protection, Inc.

Tammara Estes attended the *SETAC Pellston Workshop on the Application of Uncertainty Analysis to Ecological Risks of Pesticides* from February 24 through March 1, 2002. The workshop examined probabilistic methods for quantifying uncertainty in pesticide risk assessment. Approximately 50 worldwide representatives from government, academia, and industry were invited to attend. The results from the workshop are being compiled in a book to be published by SETAC.

Got Ethics?

As a result of the recent corporate scandals and concerns about integrity in the workplace, Kim Watson, QA manager at Stone Environmental, Inc., will be conducting a training session focusing on ethics in the regulatory arena at the November 6 meeting in Waltham, MA, of the New England Regional Chapter of the Society of Quality Assurance (NERCSQA). The presentation includes the essentials of designing an effective ethics program for the cultivation and maintenance of integrity in the workplace. Discussion will encompass fraud detection and prevention.

Watson also attended the 18th Annual Meeting of the Society of Quality Assurance in October in Albuquerque, NM.

FTP Server More Secure

Stone Environmental's FTP (File Transfer Protocol) server allows clients to quickly upload and download files that are too large for e-mail, such as draft and final reports. With increased danger of attack from the Internet, the computer staff at Stone has introduced encryption technology and other security upgrades, such as stricter file-level access control, to the FTP site's structure and organization.

Scrambling Names and Passwords

The use of encrypted FTP servers is rapidly expanding across the Internet to address security issues. The most serious vulnerability occurs when users log on to an unencrypted (traditional) FTP site: their user names and passwords are transferred "in the clear" across the Internet to the FTP server. Any possible attacker connected to the Internet between a user's computer and the FTP server can "watch" the network traffic and view the user name and password as they go by. Once attackers have a user name and password for a system, they can easily infiltrate that system. On the other hand, if the user name and password are encrypted, attackers can still see that data is being sent from the user's computer to the FTP server, but they can no longer see the actual name and password.

Clients interested in scrambling their FTP log-in information need to obtain new FTP software. Clients who do not require extra security at this time need not change anything—Stone will continue to support their current FTP software.

New FTP Software

Users who wish to take advantage of FTP encryption need to use a new software package similar to, but incompatible with, the older, traditional FTP client software. The new software is called SFTP (for Secure FTP), and it is as easy to use as the older FTP products. Just like FTP, SFTP is a computer protocol rather than a single product. As such, it enables many programs to be used as an SFTP client. One very nice Windows SFTP client product is free for evaluation and available on Stone's Web server at *http://ftp.stone-env.com/pub*. Simply download the file named *SSHWinClient-3.1.0-build235.exe*. For more information about that SFTP client, go to the manufacturer's Web site at *http://www.ssh.com/products/ssh/for_workstations/*.

Web Access to FTP

In addition to increasing security, Stone added another feature to the FTP server to enable clients to access their files using a Web browser. Clients will still have to use some kind of FTP software to upload files to our server, but it will not be required in order to download files. This new option is currently unencrypted and suffers from the same security weakness that traditional FTP does, but plans to encrypt it are in the works. Until then, this option for access to the Stone site should not be used if security is of key concern.

For more information, contact Melissa Hayden at mhayden@stone-env.com.

Stone Sails Through EPA Audit

EPA conducted a Good Laboratory Practices (GLP) inspection at Stone Environmental, Inc. in Montpelier, VT, from June 18 to 21, 2002. The inspection team reviewed the facility's compliance status with FIFRA GLP regulations at 40 Code of Federal Regulations (CFR) Part 160, as well as several studies performed by Stone.

The purpose of the audit was to validate data in final reports that Stone's clients presented to EPA in support of registrations under FIFRA. In addition, the compliance review determined whether the GLP regulations of FIFRA were being observed in Stone's testing facility's procedures and practices.

The EPA auditor reported "No Observed Adverse Findings." This is the best possible finding for this type of audit and was cause for celebration at Stone. "I made a big deal about it because it is the ultimate acknowledgment that all the hard work our staff has put in over the years to adhere to the GLP standards has been worth it," said Kim Watson, Stone's QA manager.

Stone on the Move

After 10 years of expansion, Stone has outgrown its office in the renovated school building overlooking the golden dome of the Vermont capitol building. An exhaustive search for new space landed 10,000 square feet in the newly constructed River Station Building on Stone Cutter's Way, ideally situated between the Winooski River and the Montpelier bike path. Stone's future home offers a 60 percent increase in office space, as well as more room for archive storage. The move is tentatively scheduled for January 2003, so stay tuned for a change-of-address notice.

Corn Herbicides *From page 1*

August produced concentrations of herbicides (atrazine, alachlor, metolachlor, and cyanazine) as high as those in the previous two spring runoffs (Goolsby et al., 1993).

Watershed Characteristics

Past studies also found that the runoff curve number, soil hydrologic group, watershed area, percentage of agricultural land, and herbicide use in a watershed can affect herbicide concentrations and loads in rivers.

A slight correlation of runoff curve number and herbicide concentration was shown in various watersheds in Indiana (Homes et al., 2001). Soil hydrologic group (a variable that determines the runoff curve number) was also correlated with herbicide concentrations (Battaglin and Goolsby, 1996; Larson and Gilliom, 2001).

Many studies documented inverse relationships between watershed area and concentrations of some, but not all, herbicides (Battaglin and Hay, 1996; Larson and Gilliom, 2001).

Land use was directly related to herbicide loading. Studies found that watersheds with a smaller percentage of agricultural land planted in corn had much lower unit-area herbicide loads (Richards et al., 1996; Hainly and Kahn, 1996).

Not surprisingly, there were strong correlations between herbicide use and annual mean herbicide concentrations in watersheds in the midwestern US (Battaglin and Goolsby, 1996). A more recent regression model study showed that herbicide use intensity (use per watershed area) was the best predictor variable for atrazine, metolachlor, cyanazine, alachlor, and trifluralin concentrations, with atrazine having the most effective response (Larson and Gilliom, 2001).

Stone's Findings

Stone's study compared three watersheds during one season to determine which was the most vulnerable based on different variables. Streamflow was a factor, but the most significant predictor of vulnerability was the acreage of corn planted.

References are available at www.stone-env.com/newsltr.html.

Community Water Systems Tighten Security After 9/11:
Surface Water Studies Affected

The September 11, 2001, terrorist attacks dramatically focused attention on the vulnerability of America's infrastructure, including community water systems (CWSs). The CIA put metropolitan water systems on alert for potential terrorist attacks, and in mid-July, 2002, the FBI issued a warning to water utilities after arresting Al Qaeda operatives found with documents pertaining to water security. In response, CWS managers are taking measures to safeguard their facilities and prepare for future emergencies—measures that Stone Environmental, Inc. fully supports, but that have caused some adjustments in how its scientists conduct surface water studies.

Following September 11, Stone began a yearlong surface water monitoring study. The field phase involves the direct collection of raw and finished surface water samples at community water systems across the country. Stone quickly found it challenging to access water supply data from CWS operators and state agencies because of heightened security.

States Are Requiring Written Requests, Giving Less Information

State agencies are less willing than they previously were to provide Stone with a list of community water systems that rely on surface water as their source. Written requests are now the norm, and even after they grant permission, most states will no longer release the latitude/longitude coordinates of system intakes. Also, photographing intakes and plant facilities is now forbidden at many sites.

[Editor's note: I found a photograph on the Web site of a large CWS and wrote for permission to use it to accompany this article. A CWS representative wrote back and asked me to please tell her where on the Web site it was located so that she could find and remove it. It need hardly be said that permission to use the image was not granted.]

For example, after requesting data from the Wisconsin Bureau of Drinking Water and Groundwater, Stone was required to agree that the information would be used only for the intended purpose of the study, and would be provided only to the client and the US EPA. Stone also had to agree to destroy or return the information when it was no longer needed.

The fence surrounding this storage tank was built after 9/11/2001 to tighten security at one of Vermont's community water systems.

North Dakota would not release CWS information without a written statement of who was making the request, what the reason was for it, how the information was to be used, and who would have access to it. In order for Stone to obtain CWS data from the Illinois EPA, a Freedom of Information Act request was necessary. New Jersey provided information without requiring a written request; Indiana refused outright.

Operators Still Cooperating

Once Stone obtained the data and selected the systems that met the study criteria, Staff Scientist Nell Fraser found CWS managers and staff just as willing as in the past to collect samples, despite working additional hours to conduct vulnerability assessments and prepare emergency response plans to comply with the new Public Health Security and Bioterrorism Response Act. "Even though they're busier now, we make it so easy for them to take the samples that most are still saying 'yes,'" said Fraser. "We haven't seen a decline in the participation rate." Also, the CWS operators receive the pesticide data. "They want to know about their drinking water," Fraser added. "That is a real motivator for them."

Stone is responding to the additional paperwork and restrictions by adopting more formal methods and anticipating longer turnaround times for obtaining permissions and data. "We have not had to charge clients more, or push out any deadlines," said Susan Alexander, FIFRA group leader. "We've just had to adjust our process." When states will not provide some or all of the information needed for a study, Stone turns to its in-house databases created from past studies, or EPA lists and other databases. "We've been able to find enough systems that qualify," Alexander added. "It just takes a little more effort."

For more information, contact Susan Alexander at salex@stone-env.com.

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Update of CropQuery® ArcView Extension Now Available

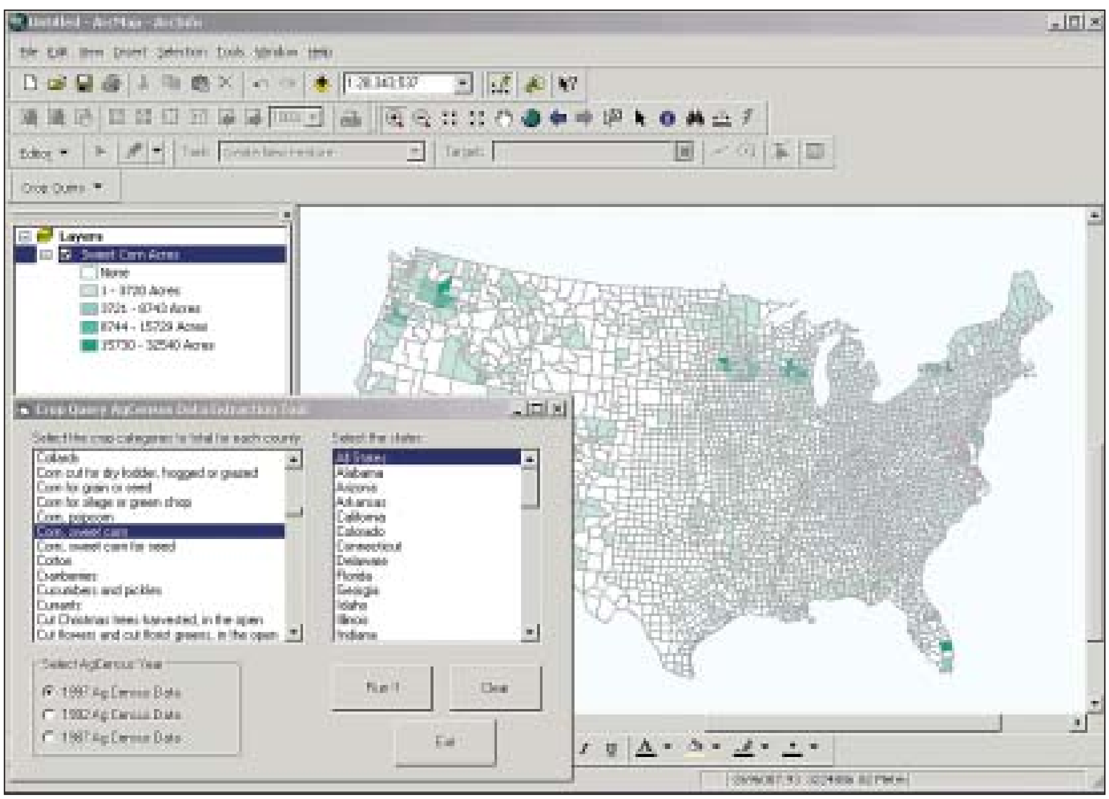
Stone Environmental has just released an update of its CropQuery® ArcView extension that is compatible with ArcGIS 8.2. The new version was developed by Stone using ArcObjects, a programming technology recently introduced by ESRI (Environmental Systems Research Inc.). Other enhancements to the new version include an automatic zoom to the user's study area and faster performance.

CropQuery® provides a clear and instant view of crop locations and areas for all counties in the United States. Users can select one or more crops in any number of states and produce quick views into current and historic crop acreage information. In addition to helping Stone with its projects, CropQuery® is a useful tool for scientists, marketing specialists, government agencies, and students.

The statistical information in CropQuery® was compiled from the USDA's National Agricultural Statistics Service's 1997 Census of Agriculture, released in June 1999 on CD-ROM. The crop data, combined with spatial county boundary information, is displayed visually using ArcGIS, ESRI's most advanced desktop GIS software product. In addition to the 1997 data, CropQuery® interfaces with historical crop data from 1992 and 1987 compiled by the Department of Commerce's Economics and Statistics Administration, Bureau of the Census. Stone will include the 2002 agricultural statistics from the USDA in CropQuery® as soon as they are available.

CropQuery® can be purchased for $495. Owners of the ArcView 3.2 extension can upgrade for $295. The CD-ROM contains all the data and ArcGIS extension files to display the crops of interest or to generate a summary file that can be queried for display.

For more information, contact David Healy at dhealy@stone-env.com.



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