# Transfer and Application of Simulation Modeling in Important Environmental Problems

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# Abstract

Watershed simulation models developed by the Agricultural Research Service (ARS) and its collaborators have made significant contributions to understanding watershed processes and conservation and protection of natural resources. However, these simulation models have broader applications in important regional and national environmental problems (i.e. Superfund sites). General guidelines and specific suggestions are made to improve ARS watershed simulation modeling research and technology transfer to address these important environmental problems. An example application of simulation models at a Superfund site is used to illustrate properties of ARS watershed simulation models that would make them more useful for these applications. Benefits to ARS from cooperation with agencies and organizations responsible for remediation of Superfund sites include improved model evaluation, verification, and validation. ARS cooperation on these problems and the watershed research appropriate to help solve them would provide renewed vigor, emphasis, and recognition of watershed research.

**Keywords:** watershed modeling, continuous simulation, Superfund sites, technology transfer

# Introduction

Watershed simulation models developed by cooperative research between the U.S. Department of Agriculture – Agricultural Research Service (USDA-ARS or simply ARS), universities, and other cooperators (model developers hereafter) have been extensively applied within the agricultural – natural resources research and technology community.

The main purposes of these models in the research community include formulating and testing hypotheses, developing predictive capabilities, and transfer of the models, and the related technology, to users and cooperators in the agriculture – natural resources conservation community. These models have significantly improved our understanding of natural resource systems, and, their use has significantly contributed to conservation and protection of these resources.

However, there are broader societal concerns in which ARS and its collaborators can make significant contributions through development and transfer of their watershed simulation models.

Superfund sites listed by the U.S. Environmental Protection Agency (EPA) are important regionally and nationally. The major environmental laws governing these sites include the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA or Superfund), the Superfund Amendments and Reauthorization Act (SARA), the National Environmental Policy Act (NEPA), and the Resource Conservation and Recovery Act (RCRA). Summary and complete text versions of these, and other applicable environmental laws, are given in EPA (2003).

Protection of human health and the environment at Superfund sites can be significantly enhanced by using natural resource simulation models such as those for watershed hydrology (water quantity and quality), soil erosion, sediment transport, sediment yield, contaminant transport, and contaminant yield.

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The ARS and its collaborators could significantly benefit from transferring their models and associated technology (e.g. databases, knowledge, and documentation) to agencies and organizations responsible for remediation of Superfund sites. Application of their models to problems at Superfund sites would significantly enhance the testing and evaluation phase of model development (i.e. model verification, validation, extension to extremes, and robustness) and thereby significantly reduce expenditures and time required for ARS scientists to accomplish this phase. Successful technology transfer requires collaboration between model developers and model users. This collaboration can provide additional resources and insight during all phases of model development and transfer. Finally, successful use of ARS models and technology to help solve important national problems enhances the scientific standing of ARS and its scientists.

The main purposes of watershed simulation models used by agencies and organizations performing environmental remediation at Superfund sites include predicting source, transport, fate and impact of contaminants. Their purposes also include analysis and interpretation of monitoring data, and evaluating performance of alternative remediation alternatives. Finally, these models and their results are used to communicate with regulatory organizations, state and local governments, NGOs, other stakeholders, and the general public. Therefore, the models and the results of applying them are subject to peer review, regulatory review, and public review.

#### Purpose, scope and limitations

This paper reviews selected properties of models that enhance their transferability, discusses some specific examples, and makes recommendations for improving the models and how they are developed and transferred. These recommendations span the entire process from basic research to technology transfer and application and to user feedback necessary to maintain a strong simulation modeling research and development effort. The example used to support broader ARS involvement in environmental problems is for the Rocky Flats Environmental Technology Site (RFETS) in the semiarid western United States. Finally, conclusions and recommendations given herein are based mostly upon the author's experiences as a consultant to agencies and their contractors (model users hereafter) at DOE Superfund sites using watershed

simulation models. These simulation models have emphasized hydrology, soil erosion and sediment yield, and contaminant transport due to runoff and erosion and thus were limited to a subset of modeling needs at Superfund sites.

#### Models Used in Environmental Remediation

As stated above, models used in Superfund site environmental remediation function as predictive tools, data and uncertainty analysis tools, alternative evaluation tools, and, communication tools. In these uses the models are subject to extensive peer, regulatory, and public review. The following sections describe some characteristics or properties these models should have to be successful for these uses.

#### Scientific credibility

Scientific credibility is crucial to model users, regulators, and the public accepting models and their results. In this user-regulator-public arena (simply user arena hereafter), scientific credibility is established by peer-reviewed publications, documented peer review of the site-specific applications, reasonableness of the results, and the ability to communicate them. A big part of this acceptance by the users is previous acceptance of the models in similar applications. Model developers should document the models and their applications in the scientific literature.

# Presentation of results

Modeling results and output must be understandable in the user arena. A critical part of most model applications at Superfund sites is spatially distributed results. The problems usually involve contaminants spatially distributed in the environment and the model results should directly address spatially distributed processes and results. Model developers attacking spatially distributed processes should adopt geospatial referencing early in model development activities. Practically, this means models should be developed and implemented in a geographic information systems (GIS) environment.

#### **Continuous simulation**

Continuous simulation means that the models simulate processes during and between precipitationrunoff events. This is necessary to calculate a water balance. For example, evapotranspiration processes continue between events and can deplete soil moisture affecting the amount of infiltration, runoff, soil erosion, etc. when an event does occur. In addition, hydrologic processes such as evapotranspiration, deep percolation and groundwater recharge/discharge occur continuously, sometimes at rates far slower than those that occur during a storm event. Therefore, continuous simulation models are required to compute a water balance, calculate low flows, calculate watershed yields, and thus contaminant loadings.

#### Evaluation of alternatives and uncertainty

The goal of environmental remediation is to change the system. This means that models must have the ability to predict site performance into the future. Models are used to quantify and predict contaminant transport pathways (surface water migration, ground water migration, air migration, biological transport) and contaminant inventories (especially in soil and water). These evaluations and predictions are made for the initial existing conditions and then for alternative remediation scenarios designed to change the pathways and inventories to reduce contaminant impacts on human health and the environment. Therefore, models most useful in the user arena should be designed to evaluate the impacts of land use and management practices (including landscape reconfiguration) alternatives, to quantify their differences and to quantify prediction uncertainty. Understanding and specifying uncertainty is critical to evaluation of alternatives. The desired changes must exceed the uncertainty bounds in contaminant transport and inventories if the proposed alternatives are to be judged different than the existing conditions.

#### **Reasonable results**

Modeling results must be reasonable. And, the criteria with which the results are judged reasonable vary between the model users, the regulators, other stakeholders, and the general public. Model results must "match" empirical data to the extent possible. Matching, in the context of users and peer reviewers, is statistically preserving the means, uncertainty, and trends in space and time. Models must also give reasonable results at the extremes – for small events and for large events. Matching, in the context of the general public, means meeting their expectations as well as those of the users and peer reviewers with regard to how well the model reproduces measured data and trends.

Model developers should thus test and document model performance across a broad range of inputs and conditions to make sure the models are robust as they "match" empirical data. Many of the users require the ability to predict contaminant concentrations under extreme conditions (low flows, floods, high winds, etc.) as well as long-term yields of water, sediment, and contaminants. These applications require continuous simulation.

#### Example of Models Used at a Superfund Site

The Rocky Flats Environmental Technology Site (RFETS) is located in Golden, CO. It is a former site of production of nuclear weapons components as part of the DOE weapons complex. Contaminant spills and subsequent transport by wind and water erosion have resulted in environmentally dispersed radioactive contaminants. The site is being remediated to meet federal, state, and local regulations by reducing offsite transport of contaminants to below regulatory limits. The following sections list the simulation models used and some of their characteristics.

#### Site-wide water balance

The model chosen to calculate a water balance was MIKE-SHE, a model developed by the Danish Hydraulic Institute (DHI) to simulate the land phase of the hydrologic cycle (e.g. see Storm and Refsgaard 1996, DHI 2003). This model is continuous, couples surface water and groundwater, and operates on a spatial grid. Key features leading to its selection (selection features) were its dynamic operation, continuous simulation, coupled surface and subsurface flow calculations, spatial operation, and its reputation as a "state-of-the-art" model. It also had good graphic presentation capabilities.

#### Wind erosion and contaminant transport

The wind erosion model was developed by contractors at RFETS because existing models were judged as inadequate. Key development features included its dynamic operation, continuous simulation, coupled sediment and contaminant simulation, and its spatial adaptation to the RFETS.

#### Water erosion

The Water Erosion Prediction Project (WEPP) model (Laflen et al. 1991, USDA-ARS-NSERL 2003) was chosen to compute upland soil erosion. The WEPP model has continuous and single storm options, simulates at the hillslope scale, and has options for cropland and rangeland applications. Key features of the WEPP model leading to its selection include its ability to operate in a continuous simulation mode, its ability to simulate erosion on complex hillslopes (multiple overland flow elements), its calculation of sediment yield from hillslopes by particle sizes (and thus the ability to compute enrichment ratio for subsequent contaminant transport calculations), and its reputation as a "state-of-the-art" model.

#### Sediment transport

The model chosen to calculate sediment transport was the HEC6T Model (Thomas 2002, MBH 2003), a proprietary modification of the HEC6 model. The HEC6T model is a one dimensional sediment transport model. Key features leading to its selection included its ability to compute non-uniform flow (backwater at constrictions, drawdown at over falls, etc.), sediment transport by particle size distribution, sub-critical, critical, and super critical flow options, calculation of channel degradation or aggradation (mobile bed hydraulic calculations), and its reputation as a "state-of-the-art" model.

#### **Contaminant transport**

The "Actinide Mobility Calculations" model was developed by contractors at RFETS because existing models were judged as inadequate. Key features developed in this model included its ability to use WEPP output (sediment yield by particle size distributions and enrichment ratios), its ability to provide contaminated sediment input to the HEC6T model, and its spatial adaptation to the RFETS.

# Discussion

Simulation modeling at RFETS was required to meet several objectives. The RFETS model users required the ability to predict water balance, soil erosion, sediment transport, sediment yield, and contaminant concentrations under extreme conditions (low flows, floods, high winds, etc.). The users also needed to predict long-term yields of water, sediment, and contaminants under alternative Site management scenarios. These requirements could be met using models that used continuous simulation. The models described above were integrated at the watershed scale to meet the user requirements.

The RFETS model users also needed models that met the criteria listed earlier, i.e. scientific

credibility, spatially distributed computations, robustness, and reasonableness of results.

#### **Developing Models to Meet User Needs at** Superfund Sites

We have already discussed many things the model developers should do to meet users' needs, but these, and additional recommendations need to be formalized and described with sufficient specificity to provide guidelines. The following partial list of model requirements is designed as a starting point for model developers:

- Obtain peer review at all steps in model • development,
- Document the models in peer-reviewed • scientific publications,
- Develop, operate, and present the models in a GIS environment,
- Use spatially distributed data, starting with • digital elevation models (DEMs) and including topography and drainage channels, soils, vegetation, and land use and management should be included as part of the model parameterization process and it should be automated in the GIS environment,
- Formulate the models to be robust; they • should operate properly for the means as well as the extremes.
- Produce predictions of means, extremes, • annual yields, and their uncertainties,
- Base the models on continuous simulation. rather than individual events only, to enable calculations of watershed yields and contaminant loadings,
- Automate uncertainty analysis within the • models, and
- Develop models that include procedures to • manage metadata, input/output databases, and to generate reports containing the metadata and documenting input/output for archiving.

# Recommendations

The ARS Strategic Plan states that a major goal of ARS research is to "increase the long-term productivity of the United States agriculture and food industry while maintaining and enhancing the natural resource base on which rural America and the United States agricultural economy depend." A major strategy to help accomplish this goal is to

"develop new concepts, technologies, and management practices that will enhance the quality, productivity, and sustainability of the Nation's soil, water, and air resources." Finally, a performance goal to help accomplish the above goals is to "experimentally demonstrate the appropriateness of watershed-scale technologies and practices that protect the environment and natural resources (ARS 2003)."

The following recommendations are specific to the Agricultural Research Service and its collaborators responsible for developing and technology transfer of natural resource (watershed based) simulation models as stated in the above goals. My experience has been with hydrologic (including quantity and quality), soil erosion, sediment transport, sediment yield, and contaminant transport and yield models. However, development and transfer of other models such as landscape evolution, interaction of biotic and abiotic processes, and ecosystem sustainability might also benefit from the following recommendations.

These are high level recommendation for ARS. Lower level detailed steps and recommendations are contained earlier in the body of this text.

The ARS should develop a conceptual model of watershed simulation modeling from initial concepts to technology transfer that includes model users and stakeholder inputs at all stages in the process. This conceptual model could be used to communicate goals and strategies from the ARS Strategic Plan to its scientists, cooperators, model users, and stakeholders and thereby enhance technology development and transfer.

The ARS watershed research centers and experimental watersheds are unique and should provide a basis to expand their cooperators and stakeholders to include those involved in important regional and national environmental problems. Cooperation on these problems and the watershed research appropriate to help solve them would provide renewed vigor, emphasis, and recognition of watershed research. A key objective should be to cooperatively develop and transfer the simulation models so vital in protecting our environment and thereby conserving our natural resources.

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