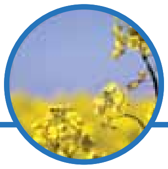
Biofuels and water quality: challenges and opportunities for simulation modeling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Quantification of the various impacts of biofuel feedstock production on hydrology and water quality is complex. Mathematical models can be used to efficiently evaluate various 'what if' scenarios related to biofeedstock production and their impacts on hydrology and water quality at various spatial and temporal scales. Currently available models, although having the potential to serve such purposes, have many limitations. In this paper, we review the strengths and weaknesses of such models in light of short- and long-term biofeedstock production scenarios. The representation of processes in the currently available models and how these processes need to be modified to fully evaluate various complex biofeedstock production scenarios are discussed. Similarly, issues related to availability of data that are needed to parameterize and evaluate these models are presented. We have presented a vision for the development of decision support tools and ecosystem services that can be used to make watershed management decisions to minimize any potentially adverse environmental impacts while meeting biofeedstock demands. We also discuss a case study of biofeedstock impact simulation in relation to watershed management policy implications for various state and federal agencies in the USA.

In recent years, high US fuel and energy prices and national security concerns have prompted a renewed interest in alternative fuel sources to meet increasing energy demands, particularly by the transportation sector. Policy signals from the current US administration now point towards sustainability of biofuel production. The Energy Independence and Security Act of 2007 (EISA) is projected to have long-term impacts on US agriculture by establishing a mandatory renewable fuels standard (RFS) requiring fuel producers to use at least 36 billion gallons of biofuel by 2022. Although corn-grain ethanol currently plays a significant role in meeting this goal, corn-grain ethanol production is capped at 15 billion gallons, with the remaining 21 billion to be obtained from cellulosic ethanol and other advanced biofuels [1]. The EISA Section 204 requires federal agencies to report to Congress, in no later than 3 years, environmental concerns associated with biofuel production using a set of science-based indicators such as air quality, effects on hypoxia, pesticides, land productivity, soil quality, water-use efficiency and water quality [1].

One of the biggest challenges in meeting the US biofuel goal is supplying large quantities of lignocellulosic materials for the production of biofuels that are produced in an environmentally sustainable and economically viable manner. Feedstock selection will vary geographically based on regional adaptability, productivity

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Key terms

Biofeedstock: Plant-derived material that can be converted to forms of fuel or energy product

Hydrology: Study of the distribution of water and its constituents through the hydrologic cycle

Hydrologic/water-quality model: Computer-based program used to estimate the distribution of water and pollutant transport associated with physical systems and hydrologic processes in representative fields, watersheds and basins

and sustainability. Changes in land use and land management practices related to **biofeedstock** production may have potential impacts on water quality [2–4]. Addressing biofuel production sustainability requires scientific assessment of regional feedstock production impacts on water quality and quantity, sediment, pesticides and nutrient losses [2]. These natural resource concerns should be carefully identified so that appropriate plans can be implemented to safeguard against or mitigate any potential adverse environmental consequences to natural resources.

The introduction of second-generation biofuel feedstocks, such as corn stover (*Zea mays* L.) [5–7], switchgrass (*Panicum virgatum* L.), miscanthus (*Miscanthus giganteus*) and fast-growing woody crops (e.g., hybrid poplar), have the potential to influence the fate of nutrients, pesticides and sediments within the environment [8]. The production of these biofeedstocks may also alter **hydrology** and water balance [9]. While some feedstock-production systems may have detrimental hydrologic and water quality impacts, others may be neutral relative to current cropping and land management systems, while others may actually improve water quality. Sustainability of these feedstock-production systems may be constrained by availability of water and current land-use activities [2]. For example, it is anticipated that corn-based feedstocks may play a significant role in the midwest USA while rice and wheat straw may be used as potential feedstocks in the southeast USA along with other aforementioned feedstocks. Researchers have suggested that crop residues improve soil productivity and the long-term impacts should be examined for its use to be justified [4]. The use of crop residue must take into account concerns that residue removal could increase erosion and reduce crop productivity by depleting soil nutrients [6], unless farmers increase fertilizer application rates to maintain crop productivity. Generally, corn residues remain on fields following harvest, thereby playing a critical role in erosion control and nutrient cycling, as well as improvement of the physical properties of soil [4].

Indepth studies are needed to quantify the specific effects of feedstock production so that appropriate watershed-management decisions can be made. Computer simulation models can serve as an effective tool to quantify the effects of biofeedstock production on hydrology and water quality at various spatial scales ranging from individual fields to watersheds and large river basins, and temporal scales ranging from individual storm events to annual and decades. These models offer capabilities to simulate various 'what if' questions related to the impact of biofuel crop production [3]. When properly implemented, the results from such models can help identify negative environmental impacts, evaluate various management practices that can be implemented to minimize those negative impacts, while quantifying the water quality benefits related to other biofuel crop production. These models can play a significant role in developing watershed-management strategies to meet biofuel crop production goals with minimum negative environmental impacts. However, the current capabilities of such models in effectively simulating hydrologic/water-quality processes related to various biofuel crop-production systems should be carefully reviewed before they are implemented to develop such strategies. The potential for different biofeedstocks, crop and land-management options, and associated rapidly changing land uses, present challenges to using existing models in making watershed-management decisions.

The overall objective of this paper is to review the strengths and weaknesses of currently available computer simulation models in light of short- and long-term biofeedstock production scenarios. We discuss the representation of processes in the currently available models and how these processes need to be modified to fully evaluate various complex biofeedstock production scenarios. Similarly, issues related to availability of data needed to parameterize and evaluate these models are discussed. A vision is presented for incorporating ecosystem service valuation in these models and how such capabilities, when embedded within a web-based decision support tool, can potentially increase the utility of these models in making watershed-management decisions. Finally, a brief case study is presented to illustrate the potential usage and limitations of a **hydrologic/water quality model** in evaluating second-generation biofeedstock-production impacts on the environment.

Hydrologic/water quality models that have been used specifically to evaluate the impacts of US biofeedstock production on water availability and water quality include:

- Groundwater Loading Effects of Agricultural Management Systems and National Agricultural Pesticide Risk Analysis (GLEAMS-NAPRA) [10–12];
- Environmental Policy Integrated Climate (EPIC) [13];
- Agricultural Policy/Environmental Extender (APEX) [14];
- Soil and Water Assessment Tool (SWAT) [15].

It should be noted that the intent of this paper is not to provide a review of all currently available models that can be potentially used to evaluate the impact of biofuel crop production on hydrology and water quality. Given the widespread interest in this subject matter, new model applications are expected to increase significantly in the future using both mechanistic (e.g., the CENTURY application) and heuristic models [16,17]. Many more models are available and have been widely used to evaluate hydrologic and water quality impacts of land use and land management at point, field and watershed scales. Migliaccio and Srivastava [18] as well as Borah and Bera [19] have provided good reviews of the hydrologic process representation in potential models, some of which are not highlighted in this paper. Similarly, Srivastava *et al.* have presented an overview of water quality processes in potential hydrologic/water quality models and should be consulted for additional details [20]. We have focused our discussion on biofeedstock production in agricultural systems. We recognize that many other feedstocks, such as algae, can potentially play a significant role in meeting biofuel production goals; however, discussion of the hydrologic/water quality impact simulation of such feedstocks is beyond the scope of this paper.

Overview of hydrologic/water quality models used to evaluate the impact of US biofeedstock production

In general, the choice of model depends on the problem at hand and the overall project goal [21]. Once a specific problem has been established and it has been determined that a modeling approach could address such a problem, the decision model selection should be made on the basis of model accuracy, simplicity, consistency and sensitivity [21,22]. Researchers have used the GLEAMS-NAPRA, EPIC, APEX and SWAT models to address 'what if' scenarios related to the environmental impacts of US biofeedstock production. In addition to meeting the criteria of model selection, the aforementioned models discussed in this paper were selected due to their similarity to many existing field- and watershed-scale deterministic models used for the hydrologic assessment of agricultural systems.

▪ GLEAMS-NAPRA model overview

The GLEAMS model can simulate the edge-of-field and bottom-of-root-zone loadings of water, sediment, pesticides and plant nutrients [10]. Hydrology, erosion, nutrients and pesticides are major components of the GLEAMS model. These components can simulate the effects of cropping systems on surface- and ground-water quality on a daily basis utilizing climate, soil and management data inputs [10]. The NAPRA tool has been used to evaluate the effects of agricultural management systems on surface and subsurface water quality [11]. NAPRA uses GLEAMS as a core model to simulate surface runoff, percolation, erosion, pesticide and nutrient losses with similar user input requirements (Table 1).

The hydrology component of the model is based on the modified US Department of Agriculture (USDA)-soil conservation service (SCS) curve number (CN) procedure and a soil moisture-accounting technique that considers moisture depletion as influenced by rainfall and evapotranspiration [23]. The model uses CN only at the beginning of the simulation process and incorporates various hydrological processes, such as infiltration, runoff, soil evaporation, plant transpiration, rainfall/irrigation, snow melt and soil water movement, within the root zone to calculate water balance [10]. GLEAMS does not use CN to calculate daily runoff, but uses CN to estimate a maximum storage volume. GLEAMS calculates a daily soil water content from the previous day minus actual evapotranspiration to estimate the soil water content [24]. Soil physical properties such as porosity, field capacity, wilting point and initial abstraction, along with soil water content are used to estimate the runoff, percolation and new soil water content [24].

The GLEAMS-NAPRA model was used to evaluate impacts of first-generation biofeedstock production (corn grain ethanol) scenarios on hydrology and water quality [3]. This study quantified the long-term water quality impacts of projected cropping system shifts associated with increased demands for grain-based biofeedstocks for ethanol production. The researchers suggested that increasing demands for biofuels could result in increased usage of fertilizer and pesticides as well as increased water quality degradation from losses of associated nutrients and chemicals [3]. The results showed that agricultural management decisions involving a shift to continuous corn cropping would greatly impact estimates in erosion, fungicides and phosphorus losses from agricultural fields. This could potentially have greater impacts on runoff losses of those pollutants compared with the projected changes in crop rotations alone [3].

▪ EPIC & APEX model overview

The EPIC model [25], also known as the Environmental Policy Integrated Climate model, can be used to assess field-scale effects of agricultural management systems [26]. The EPIC model has nine components: weather, hydrology, erosion, nutrients, soil temperature, plant growth, plant environment control, tillage

Table 1. Summary of model inputs and outputs for the GLEAMS-NAPRA, EPIC, APEX and SWAT models.

Model	Model inputs†	Outputs
GLEAMS-NAPRA	Climatic inputs: precipitation, maximum and minimum temperatures, dew point temperature, wind speed and solar radiation	Hydrologic output: surface runoff, percolation and evapotranspiration
	Field inputs: soil physical and chemical characteristics (NASIS database) slope and field length and USLE C-factor	Pollutant: soil erosion, nitrate–nitrogen, soluble P, sediment P, total P, ammonia and pesticide concentrations
	Management inputs: crop type, tillage type and dates, planting, maturity and harvesting dates Fertilizer type (inorganic/manure), application date, rate and method Pesticide name, application method, date and rate	Crop related output: harvested crop yield, above surface residue and root residue
EPIC and APEX	Climatic inputs: precipitation, maximum and minimum temperatures, relative humidity, wind speed, solar radiation Management inputs: crop type, tillage type and dates, planting, maturity and harvesting dates, harvest efficiency. Fertilizer type (inorganic/manure), cost, application date, rate and method Pesticide name, cost, application method, date and rate	Hydrologic outputs: surface runoff, crack flow, subsurface flow, tile flow and lagoon overflow Pollutants at subarea or watershed outlet: pesticides concentrations, sediment losses, wind erosion nitrate–nitrogen losses (runoff, subsurface flow and leaching), soil organic carbon, carbon dioxide nitrogen (ammonium, nitrate and organic) and phosphorus (soluble and adsorbed/mineral and organic)
SWAT	Climatic inputs: precipitation, maximum and minimum temperatures, relative humidity, wind speed and solar radiation Land use inputs: HRU's: cropland, pasture, forest, urban. Management inputs: crop type, tillage type and dates, crop planting, maturity, and harvesting dates and harvest efficiency Fertilizer type (inorganic/manure), application date, rate and method Pesticide name, application method, date, rate, and harvest efficiency	Hydrologic outputs: surface runoff, ground-water flow, stream flow, crack flow and tile flow HRU level and in-stream pollutant losses: sediment yield, nitrate–nitrogen, total P, soluble P, suspended solids, ammonia, pesticide, bacteria (*Escherichia coli*), pesticides and crop yields

†Refer to models' documentation for additional details on input requirements.
APEX: Agricultural Policy/Environmental Extender; EPIC: Environmental Policy Integrated Climate; GLEAMS-NAPRA: Groundwater Loading Effects of Agricultural Management Systems and National Agricultural Pesticide Risk Analysis; HRU: Hydrologic response unit; NASIS: National Soil Information System; SWAT: Soil and Water Assessment Tool; USLE: Universal Soil Loss Equation.

and economic budgets [13]. The model has been used primarily to provide edge-of-field estimates in **soil erosion**, nutrient loss and carbon sequestration **(Table 1)** [27]. This field-scale model has undergone a series of developments and now has the capability of simulating runoff and leaching of nutrients and pesticides, carbon sequestration, wind erosion and climate change impacts on crop yield and erosion [13,28]. EPIC estimates runoff volume using a modification of the SCS curve number method, similar to the Chemicals, Runoff and Erosion Management Systems (CREAMS) model [29]. The curve number is estimated as a function of rainfall, soil type, land management and soil water content. A provision within this method allows estimation of runoff on frozen soils, with peak runoff rate based on the rational formula. The percolation component uses a routing technique to predict flow through the soil profile, governed by the saturated conductivity of the layers [25]. Soil temperature affects percolation, which ceases when soil temperature in a given layer is 0°C. EPIC accounts for lateral subsurface flow, which is partitioned with percolation and is a function of land slope and saturated conductivity. The EPIC model offers an option to use either SCS CN or the Green–Ampt equation to estimate infiltration during individual storm events [25]. There are four options for estimating potential evapotranspiration: Hargreaves–Samani, Penman, Priestly–Taylor and Penman–Monteith. Similar to the GLEAMS model, EPIC computes soil and plant evaporation separately using the Ritchie approach [25].

Key term

Soil erosion: Detachment and movement of soil from the land surface by wind or water

The APEX model [14] is a multifield version of EPIC developed to address environmental problems associated with livestock and other agricultural production systems on a whole farm or small watershed basis [30]. The APEX model structure is similar to EPIC and includes the same nine major components [31]. However, APEX has components for routing water, sediment, nutrients and pesticides across complex landscapes and channel systems to the watershed outlet and a manure management routine that supports simulation of liquid waste applications associated with concentrated animal feeding operations [30]. Powers *et al.* applied the APEX model to evaluate biofeedstock-production scenarios involving crop rotation and switchgrass production, with focus on soil and water quality in Eastern Iowa [31]. The authors concluded that achieving a sustainable approach to the production of biofeedstock crops must include aspects of total yield, water quality and soil quality [31].

SWAT model overview

The SWAT model is a physically based watershed-scale model developed to simulate hydrological processes as well as the fate and transport of nonpoint source pollutants [15]. The model has eight major components: hydrology, weather, sedimentation, soil temperature, crop growth, nutrients, pesticides and agricultural management [32]. The model operates on a continuous daily basis using soil information, land use, crop-management practices, topography and climate inputs (Table 1) [15]. SWAT divides a watershed into multiple subwatersheds with additional lumped units known as hydrologic response units (HRUs) [32]. These HRUs are composed of unique combinations of land use, soil and management practices. At the HRU level, erosion, nutrient and pesticide dynamics and water balance are computed [15]. A stream- and reservoir-routing process is then used to assess the sediment yields, total nutrient and pesticide loading and concentration at the subwatershed and the watershed outlet [15]. Field-scale process representation in the SWAT model is adopted from similar subroutines in the GLEAMS and EPIC models.

The SWAT model divides the hydrology cycle within a watershed into two components: the land phase and the channel-routing phase. The land phase controls the amount of water movement to the channels of each sub-basin, while the routing phase controls water and pollutant transport through the channel network of the watershed to the outlet. The land phase of SWAT's hydrologic cycle is based on the water-balance equation, which includes the soil water content, daily precipitation, runoff, evapotranspiration and return flow [32]. Precipitation is the primary mechanism by which water enters the land phase of the hydrologic cycle [32]. Surface runoff is estimated using either the SCS curve number procedure or the Green–Ampt infiltration method. Evapotranspiration is the primary mechanism by which water is removed from the land phase of the hydrologic cycle [32]. SWAT provides options to use the Penman–Monteith, Priestly–Taylor or Hargreaves methods to compute potential evapotranspiration [32]. Once the inputs of flow, sediment, nutrients, pesticides and bacteria from the land phase to the streams are quantified, SWAT routes the loadings through the stream and reservoir network to the watershed outlet using the routing phase of the hydrologic cycle. In addition to the mass balance of various flow and pollutant loads, SWAT also calculates transformation of chemicals in streams and streambeds.

The SWAT model has been extensively used to evaluate impacts of various land use, management and climate conditions on hydrologic and water quality response of agricultural and mixed land use watersheds [19]. There are more than 600 peer-reviewed journal articles on use of the SWAT model [101]. Gu and Sahu applied the SWAT model to the Walnut Creek watershed in Iowa to examine the effectiveness of contour strips of switchgrass in reducing nitrate–nitrogen losses from fields to rivers and lakes [33]. The study tested the hypothesis that perennial vegetation, such as switchgrass, used as a filter strip could improve water quality while potentially providing a source of biofeedstock for ethanol production [33]. Babcock *et al.* used SWAT to conduct a sensitivity analysis to identify water quality impacts of changing landscapes to crops that can be harvested for alternative energy purposes [34].

Challenges/limitations of current models in evaluating effects of biofuel crops on hydrology & water quality

Although computational models, such as GLEAMS-NAPRA, EPIC and SWAT have been used for predicting water quality impacts of biofuel crops [3,34–38], rapidly changing land use and crop-management conditions related to biofeedstock production have presented several challenges to the currently available models that can be used to evaluate the potential impacts of these changes. These challenges include:

- Insufficient data for calibration, validation and sensitivity analyses of the models;
- Crop residue management and associated hydrologic/water-quality impacts;
- Simulation of crop-management scenarios;
- Spatial and temporal process representation;
- Scaling of results from plot scales to watershed and regional scales;
- Need to quantify ecosystem services from various biofuel feedstocks;
- Availability of easy-to-use decision support tools.

Insufficient data for calibration, validation & sensitivity analyses

One of the biggest challenges involved in using current models to evaluate hydrologic/water quality impacts of biofeedstock production is the availability of measured

Key term

Energy crops: Nonfood crops grown for the specific purpose of producing liquid fuel or electricity

data related to biofeedstock crop production, management including biomass yield and nutrient/pesticide management. Such data are necessary to evaluate models and improve confidence in model predictions. Biofeedstock characteristics will strongly influence the method of harvesting and transportation, subsequently influencing how land management is represented by models. Biofeedstock crop characteristics are rapidly changing, with the development of new varieties having drastically different yields, nutrient/pesticide management and growth characteristics than available in the current crop databases. It is also expected that these characteristics will vary regionally as a function of soil and climate conditions. Lack of data representative of current biofeedstock characteristics pose challenges in performing model sensitivity, calibration and validation analyses, which are needed before models can be used to make watershed-management decisions [21]. Lack of readily available measured data is one of the most important challenges to evaluating the suitability of current models in quantifying the impacts of various biofeedstock production scenarios on hydrology and water quality.

Residue effects on hydrologic/water quality

Impacts of residue removal on water balance, erosion and nutrient/pesticide transport are not fully understood. Vegetation or residue cover generally reduces overland flow and increases infiltration. The removal of surface residue, whether completely or partially, will likely increase runoff and erosion, while decreasing infiltration. However, the magnitude of this impact is yet to be quantified and validated across different ecosystems. Generally, models redistribute portions of the above ground biomass to the nutrient pool. Removal of residue will affect soil nutrient redistribution as well as soil temperature; this could have important consequences on crop growth and nutrient uptake, with subsequent effects on nutrient losses.

The representation of biomass-production effects on erosion, in models such as GLEAMS, allows user-defined inputs and is not a dynamic process. Input values critical to erosion prediction, such as the crop cover factor (C-fact), are currently obtained externally from the Revised Universal Soil Loss Equation version 2 [39]. C-fact is a sensitive parameter in GLEAMS and its misrepresentation could have impacts on erosion losses as well as the transport of sediment-attached pesticides or nutrients [40]. Hydrologic/water-quality models could be improved by allowing dynamic association of crop residue removal with erosion, pesticides and nutrient losses. Such dynamic improvement in current hydrologic/water quality models would facilitate modeling efforts involving long-term water quality impacts in removing large quantities of biomass for biofuel production.

Crop-management challenges

There will be regional variability in biofeedstock selection due to climatic adaptability and topography. Large-scale production effects of **energy crops** such as hybrid poplar, switchgrass and miscanthus on intensively managed landscapes may not be easily represented in current models without modifications of the underlying process representations. Perennial biofuel feedstocks, such as switchgrass and miscanthus, would require an establishment phase during the first year, followed by harvest in year two onwards [41]. Herbicide and fertilizer usage would be necessary during the establishment phase of the aforementioned perennial energy crops [41]. Additionally, some tillage will be performed in year one with no tillage in the subsequent years. Typically, continuous simulation models, such as SWAT, use the first few years of simulation as model 'warm up' years to ensure that model parameters reach steady state, representing actual soil and crop conditions [42]. Hydrologic/water-quality impacts can be expected to be different during establishment phases and production phases of these perennial biofeedstocks. Crop management during the establishment phase may have important potential water quality implications. For example, a crop failure during the establishment phase may lead to greater losses of sediment, nutrients and pesticides, which may negate the positive water quality benefits during the subsequent production years. Currently available continuous simulation models, such as SWAT, need to be modified to accurately capture the hydrologic/water quality impacts during both crop establishment and production phases. SWAT assumes that annuals and perennials reach their full maturity within a single year. While the assumption holds true for annuals, perennials (e.g., switchgrass and miscanthus) may take 2–3 years to reach full growth potential. Thus, the assumption above only holds true when the crop is mature. The plant growth algorithms must be modified to model growth of perennials during the establishment phase accurately. During the establishment phase, biomass accumulation, leaf area development, canopy height and transpiration are significantly different than during the production phase. The methodology adopted in SWAT to simulate biomass accumulation in trees can be modified for perennials during their establishment phase. Once the plant has reached its full growth potential, the existing plant growth algorithms for perennials may be used. These modifications are necessary because, during the establishment phase, nutrient uptake by the plant will be much less compared with the mature phase. Thus, if the annual fertilizer application rate is kept relatively the same throughout the lifetime of the plant, there is a greater likelihood of more nutrient losses via both surface and subsurface pathways during the establishment phase than the production phase.

There are mixed results reported in the literature when nutrient and erosion losses were compared for dedicated energy crop and traditional crop production. Nelson *et al.* concluded that switchgrass production on conventional agricultural lands, in northeast Kansas, provided reductions in edge-of-field nitrate and erosion losses [37]. However, it was not clear whether or not the analysis accounted for switchgrass harvesting frequency as well as a recommendation that calls for 11.2 kg of nitrogen to be added for each ton of biomass harvested [43]. Some researchers have reported greater losses of nutrients during the establishment phase of biofuel crops. For example, the total nitrogen loss from switchgrass was much higher during the second year of growth compared with the long-term average [38]. Similar results were reported by Green *et al.* where they observed greater runoff from switchgrass in its first growing season than that from corn [44]. They partially attribute the higher runoff volume to the low transpiration from switchgrass that had lower biomass production than corn [44]. However, the modeling study by Powers *et al.* showed that, in Iowa, even with high fertilizer rates (up to 260 N kg/ha), a much lower fraction of fertilizer is lost to surface water with switchgrass than corn [31]. The long-term impacts of switchgrass on soil productivity remain unknown, due to uncertainties between fertilizer application rates and yields as well as a lack of field-measured data to quantify the fate of nutrients with surface runoff, percolation and erosion losses [45]. A current recommendation discourages fertilization usage during the establishment year, primarily to minimize weed competition, which was not accounted for in some modeling studies [46].

Additionally, the current targeted energy crops are not available in the crop databases for some models. Crop characteristics such as root depth, potential yield, ratio of nitrogen to phosphorus, carbon–nitrogen ratio at harvest and nitrogen content of crops, for example, must be obtained for each new energy crop. Numerous crops are being promoted for use as biofuel feedstocks; however, the SWAT crop database contains limited data for biofuel crops. Switchgrass is the only crop considered for cellulosic ethanol, for which parameters are available in the database. The parameters for switchgrass have been derived from yield and modeling experiments conducted by Kiniry *et al.* at various sites in Texas [47]. Kiniry *et al.* have reported different values for these parameters from experiments conducted in different parts of the USA, which have not been used in SWAT [48,49]. The database is also not representative of crops such as miscanthus and sweet sorghum (*Sorghum bicolor* L.), which are increasingly being considered as feedstock for second-generation biofuels. The parameters for these crops need to be compiled from published results or field experiments and need to be included in all watershed models.

There are other limitations associated with crop modeling using SWAT. The values of radiation use efficiency (RUE), maximum leaf area index (LAI_{mx}) and light extinction coefficient (k) are fixed throughout the simulation period. Field-scale simulations for switchgrass suggest that RUE, LAI and k can vary considerably depending upon climatic conditions [50]. SWAT uses a stress factor ranging from 0 to 1 to adjust total biomass accumulation for a given day to represent water, temperature and nutrient stresses. However, the existing algorithm can be modified to reflect changes in the growth variables rather than using a factored reduction in biomass accumulated. Grassini *et al.* have suggested a switchgrass simulation model that calculates a stress on LAI and RUE depending upon soil moisture [51]. A stress on RUE is also simulated depending upon the ambient temperature. Tahiri *et al.* have shown that transpiration in wheat is better simulated with a variable k (as a linear function of LAI) than a fixed k. Incorporation of such changes in the existing plant growth equations may better represent inter-year variations in biomass growth of crops [52].

Another limitation in SWAT is that it allows only one land cover growing in a hydrologic response unit at a certain point of time. Mixed species of grasses have shown potential for high biomass yields compared with monocultures. Simulation of such mixed systems would require changes in the current algorithms [53]. The ALMANAC model is capable of simulating more than one crop cover at a certain point in time and its algorithms may be adapted to mixed model systems in SWAT [54].

Forest biomass has been proposed as a potential feedstock for cellulosic ethanol. The water quality impacts of using forest biomass or converting existing cropland to forests need to be studied. SWAT has been used to model forests on hillside croplands in the Yangtze River watershed in China. The simulation results showed a reduction in sediment, organic P and organic N yields at the watershed level [55]. However, according to Kiniry *et al.* the forest growth algorithms of SWAT require changes to reflect the impacts of forest-management practices on hydrological processes [49]. Amatya *et al.* claim that the current version of SWAT does not simulate forest hydrology accurately and have suggested changes to the curve number method based on modeling carried out for a forested watershed in the

South Carolina coastal plain [56]. Watson *et al.* have used a modified SWAT code to model streamflow from forested watersheds in the Boreal Plain in Canada [57]. The calibration period coefficient of efficiency for daily runoff was 0.81. However, the model did not perform well during the validation period.

MacDonald *et al.* have used a modified version of the ALMANAC model and interfaced it with SWAT to simulate management practices on forested systems in the Boreal Plain of North America [54]. They simulated two scenarios on a 200-ha Boreal Plain watershed having three sub-basins. The first scenario consisted of modeling the watershed as entirely covered with mature trees. The second scenario consisted of modeling the same watershed with one of its sub-basins completely harvested. They observed that the outflow fell in the year of harvest but gradually increased with time. This suggested that evapotranspiration was being modeled satisfactorily by the SWAT–ALMANAC interface [54].

The above discussion shows that SWAT may be used to model forested watersheds and forestry-management practices with some modifications. Fast-growing trees such as poplars have shown promise as a feedstock for biofuel and a modified SWAT code may be an ideal tool to accurately predict the water quality implications of land-use change to forests.

Spatial & temporal effects

Effects of large-scale biofeedstock production can be expected to vary spatially and temporally. For example, it is expected that environmental impacts will be different during the establishment phase as compared with the harvesting phase of the biofeedstock crops. Similarly, within a given watershed, slope, soil and management characteristics will determine the impacts of these crops. Similar variability in effects can be expected at regional scales. Existing models may need to be modified and new models may need to be developed that could better represent the temporal and spatial effects of biofeedstock production on water quality.

It is expected that many of the biofeedstock crops will be grown in marginal and poor soil-quality conditions that are not suited for row-crop production. How large-scale production in marginal lands will affect hydrology and water quality is not clear and these areas are generally at greater risk of negative environmental impacts. Changes in conditions such as soil organic matter could respond at a much slower rate than expected and would affect nutrient availability in various pools. Representing this effect across multiple soils and slopes will be challenging to current models and needs to be evaluated.

Scaling of plot studies

Many of the second-generation biofuel crops are currently being evaluated at plot or small field scales. Most of the water quality data related to feedstock production comes from experiments conducted at the plot or small field scale [44,58–61]. Evaluating watershed-scale models using plot-scale data is challenging. The ability to predict watershed-scale impacts will be constrained by the ability of models to scale plot-scale data to watershed-scale impacts. These challenges will be similar to evaluating best management practice (BMP) effects. Many of the BMPs, such as vegetative filter strips, were developed using data from plot-scale studies [62]. When plot-scale data were scaled up to watershed scales, BMP effectiveness values were frequently overestimated. While plot-scale studies are appropriate for the initial understanding of production of feedstock characteristics, scaling up plot-scale results to field- or watershed-scale processes will be a key to accurately evaluating hydrologic/water-quality impacts. In the context of effective water quality-impact assessment, evaluation of nutrient losses through available pathways would require models to incorporate fate and transport of nitrogen (N) and phosphorus (P) at adequate spatial and temporal resolutions. For example, loss of N in the form of nitrate (through leaching and denitrification) and in the form of ammonia (through nitrogen immobilization in soil and subsequent volatilization) are important processes that should be represented in the modeling approach [63–65].

Coupled with the goal of representing complex biogeochemical processes is the issue of spatial optimization, where multiple scenarios of land use and other best management practices are simultaneously modeled to evaluate tradeoffs. Traditionally, to deal with the spatial representation and modeling of the heterogeneity, hydrologic models have been integrated with geographic information systems (GIS) [66,67]. However, such systems offer limited capability for data-intensive spatial optimization applications and bypass such limitations by compromising either data resolution (aggregation) or the spatial extent of analysis. Flexible and extendable geospatial information systems frameworks are needed that will allow integration and utilization of high-resolution data and models over large (regional to national) spatial extents [68]. Given that the majority of the spatial data are in a raster data model, recent efforts have focused on extending GIS with a cluster computing approach [69] as well as scalable parallel visualization [70]. Such approaches hold promise for scaling up hydrologic/water quality modeling and simulations over larger spatial and temporal scales as has been demonstrated by Whittaker [71].

Need to quantify ecosystem services to fully assess impacts of biofeedstock production on the environment

Agricultural intensification to meet food and bioenergy demands and associated land-use changes can alter various ecosystem services (ES), including provisioning services (e.g., food and energy production) and regulating services (e.g., flood, sediment, nutrient and pest regulation). These impacts may be positive or negative depending upon land-use changes associated with biofeedstock production [9]. For example, increased corn production may result in increased sediment, nutrient and pesticide losses to streams [3], while second-generation biofuel crops (e.g., miscanthus and switchgrass) may reduce the losses of sediment, nutrients and potentially enhance ES when strategically located in a watershed. To prevent further degradation of agricultural and mixed land-use watersheds, we must be able to evaluate ES and develop sustainable watershed-management strategies to maximize various ES that directly benefit humans. To date, we do not have comprehensive and easy-to-use tools that allow us to directly quantify ES from various land-use activities for effective watershed management. To address this gap, there is a need to:

- Develop decision-support tools that quantify ES and the effect of biofuel crop production on ES supply from agricultural lands;
- Estimate the economic value of key provisioning and regulating ES;
- Develop spatially explicit watershed-based scenarios to illustrate economic and environmental tradeoffs that arise across space and time.

Outputs from the individual process-based models (e.g., SWAT and GLEAMS-NAPRA) include stream flow, sediment, nutrient, pesticide losses, evapotranspiration and amount of biomass produced for various biofuel crops. However, there is no consensus on how these outputs can be converted to quantifiable provisioning and regulating ES. There is a need to develop methods for quantifying ES so that watershed-management decisions can be made to maximize these ES. When such capabilities are embedded in an easy-to-use decision-support tool (DST), watershed managers have a powerful tool to maximize both biofuel crop production and water quality benefits. Similarly, such tools can be used to evaluate how these ecosystems should be managed to improve ES from various stressors. Such analyses should provide quantitative information about thechoice and placement of BMPs needed to maximize ES while maintaining high biofuel crop productivity of these agroecosystems.

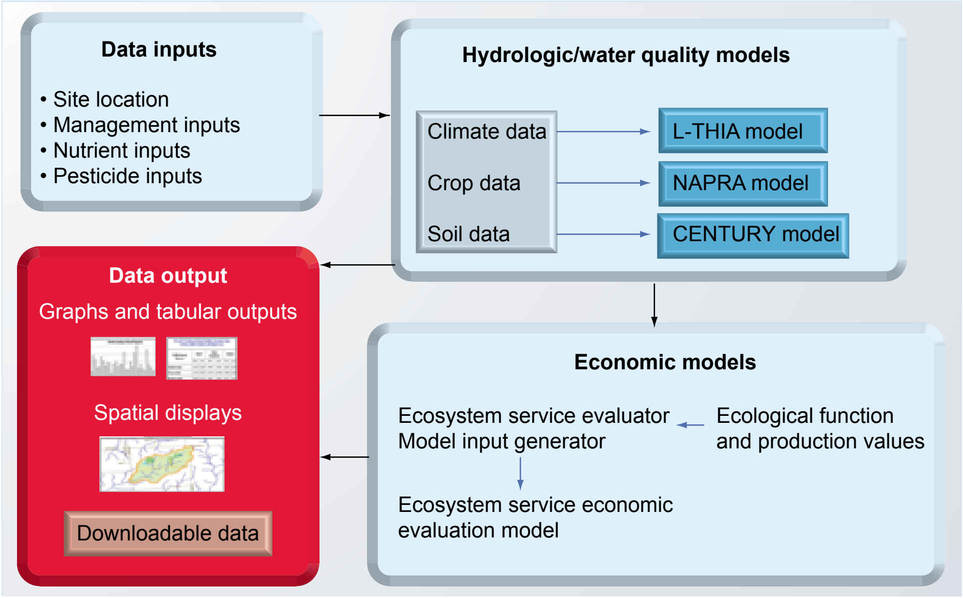

Figure 1. Decision support tool framework for quantifying impact of biofuel production on hydrology and water quality.
L-THIA: Long-Term Hydrologic Impact Assessment; NAPRA: National Agricultural Pesticide Risk Analysis.

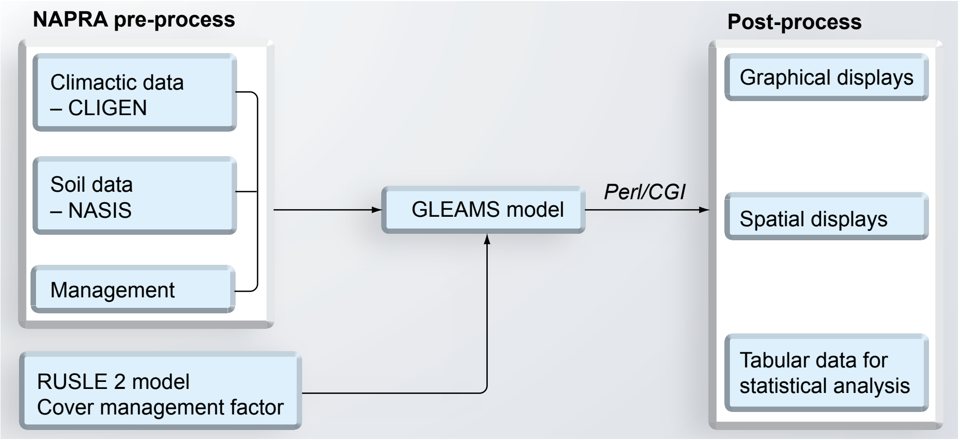

Figure 2. Modeling framework used to evaluate the impact of corn stover removal on hydrology and water quality using GLEAMS-NAPRA model.

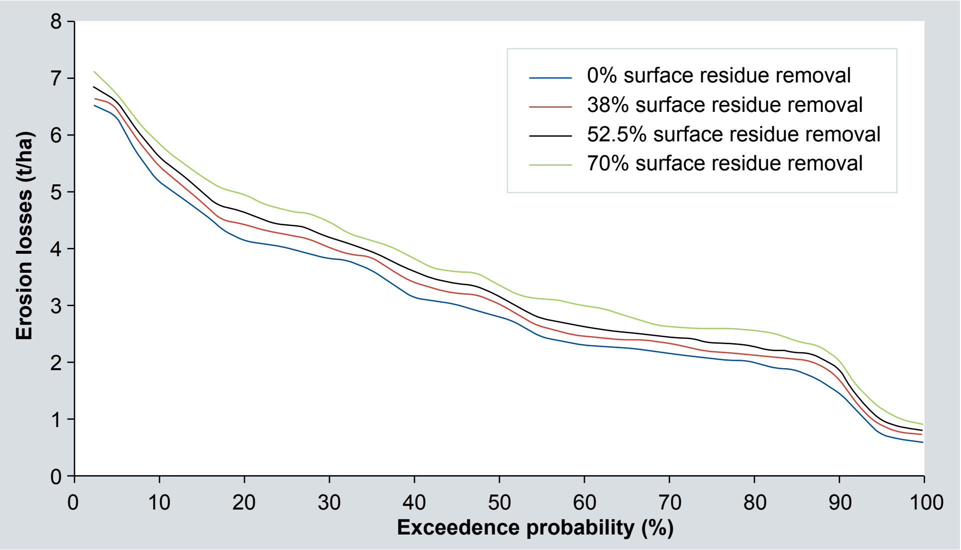

Figure 3. Estimated annual erosion losses associated with four corn-stover removal levels. Estimates were obtained from a long-term (32-year) Groundwater Loading Effects of Agricultural Management Systems (v.3.0.7) simulation on Blount Silt Loam soil (3% slope), Allen County, IN, USA.

various alternative crop-production and land-management scenarios and their corresponding impacts on hydrology and water quality. An example of such a DST framework that utilizes the GLEAMS-NAPRA model, watershed geophysical data and output visualization options is presented in Figure 1. The preprocessor in the NAPRA tool constructs GLEAMS input files from user-provided crop management, pesticide, and nutrient data in the input interface by querying databases and by running weather generator models. A post-processor within the DST framework generates the hydrology, pesticide and nutrient loss probability of exceedence. The NAPRA tool can be run for county or watershed areas to visualize the spatial variation of pesticide and nutrient losses in surface and shallow groundwater. Outputs from the DST allow quantification of surface runoff, movement of water below the rootzone, erosion and movement of pesticides and nutrients in runoff, water leached below the rootzone and with eroded soil in tabular and graphical format. Outputs can be readily connected to maps so that NAPRA results can be mapped spatially.

▪ Need for decision support framework

Current information technologies such as the internet and GIS have provided opportunities to overcome many of the limitations of computer-based models in terms of data preparation as well as visualization [72]. There is a need to develop web-based DSTs using the models described above so that stakeholders can easily evaluate

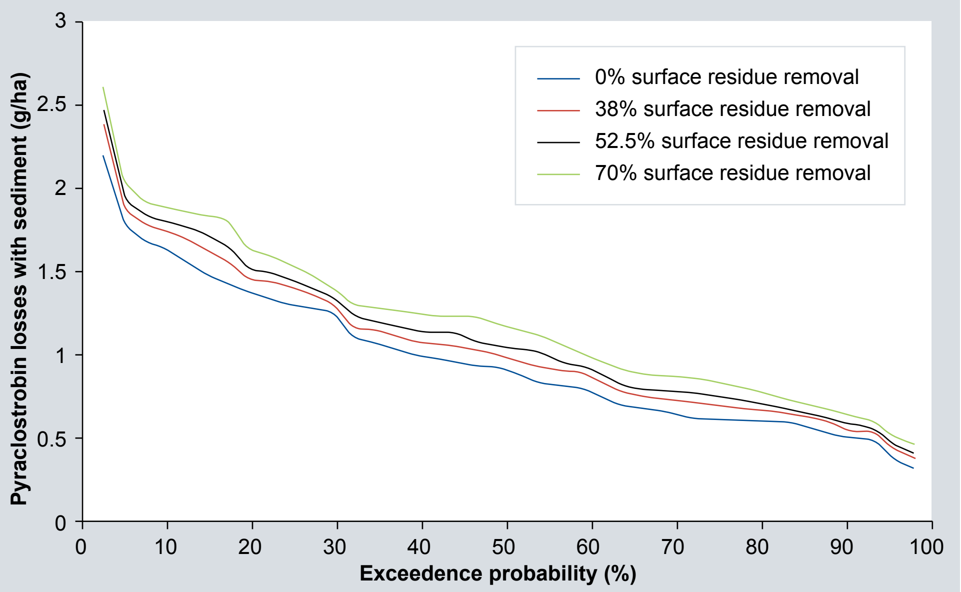

Figure 4. Estimated annual losses in pyraclostrobin (foliar fungicide) associated with continuous corn production and four levels of corn-stover removal rates. Estimates were obtained from a long-term (32-year) Groundwater Loading Effects of Agricultural Management Systems (v.3.0.7) simulation on Blount Silt Loam soil (3% slope), Allen County, IN, USA, with an application rate of 0.22 kg ai/ha.

Modeling water quality impact of biofuel crop production

▪ Case study

The case study presented below demonstrates some of the challenges faced in modeling the hydrologic/water-quality impacts of biofeedstock production. An integrated modeling approach was used to evaluate the impacts of land-management options associated with corn residue removal using the GLEAMS-NAPRA model (Figure 2). Crop residue removal rate is not a user input option with the current version (3.0.7) of the GLEAMS model. Even with modifications to the source code to represent corn-stover removal, insufficient field-related data made it impossible to calibrate and validate the model for stover removal, a desirable step to enhance confidence in model predictions.

The case study location was Allen County, northeastern Indiana. Portions of this county drain to Lake Erie, while other portions drain to the Gulf of Mexico. The county is largely agricultural (80%) and has soils and topography representative of the northern two-thirds of Indiana. A detailed description of the model, methods and datasets are presented in Thomas *et al.* [3]. Pesticide losses to surface and ground water are ongoing concerns in this region, due to potential contamination risks to public drinking water sources. Scenarios under continuous corn cropping system were examined due to the high residue production associated with that cropping system. Soybean is a low residue crop that leaves little or no surface residue in the following year and, as such, may not be a biofuel feedstock of interest. In Indiana, **corn stover**, the portion of the corn residue remaining after corn grain is harvested, is considered one of the best-suited biofeedstocks for cellulosic ethanol production based on regional transportation and economic analyses [73]. Corn stover, obtained across the USA, could potentially produce 38.4 GL of bioethanol based on an annual estimated potential yield of 130 Tg [74].

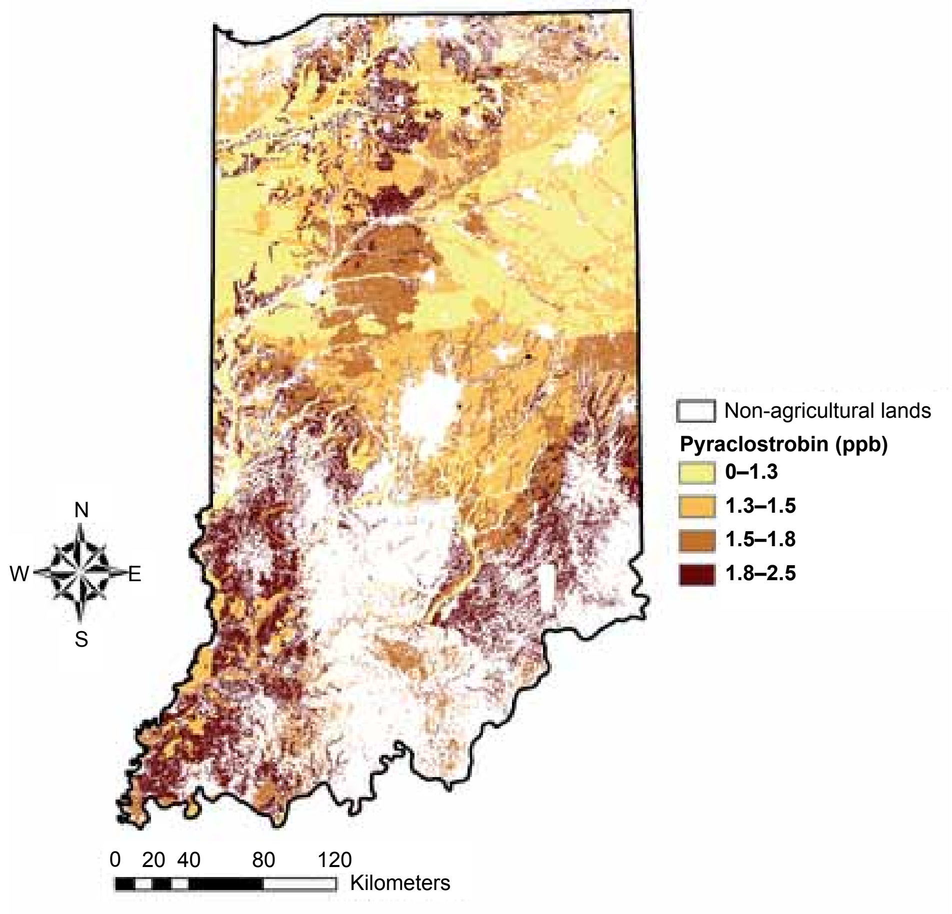

Figure 5. Long-term statewide simulated losses of the foliar fungicide pyraclostrobin from corn grain production showing regional differences in the risk to surface water.
ppb: Parts per billion.

Corn-stover removal levels were determined based on collection efficiency of typical hay equipment operating on a multipass field-harvesting technique [75]. The Indiana economic assessment study proposed the use of three corn-stover harvesting levels: 38, 52.5 and 70%. Consequently, those levels were used to compare with a benchmark of no crop residue removal (0%) with a continuous corn production on Blount Silt Loam soil. Long-term (32-year) simulations using the modified version of GLEAMS (version 3.0.7) quantified erosion, atrazine (a herbicide) loss and an emerging concern to regional water quality (runoff of foliar fungicides: pyraclostrobin, propiconazole and azoxystrobin applied to corn) [3,76].

The model results indicated that harvesting corn-stover for cellulosic ethanol production would impact annual erosion losses on Blount Silt Loam soils, with median losses of 2.82, 3.06, 3.21 and 3.39 t/ha for 0, 38, 52.5 and 70% corn stover removal, respectively (Figure 3). Model results, for a single soil, suggest that the removal of crop residue would reduce soil cover protection and, thereby, increase the potential of erosion losses to the edge of fields [3]. Whereas these estimates for erosion provided an initial understanding of residue removal impacts at the field scale, due to scaling limitations, it does not provide adequate understanding of those impacts at the watershed scale.

The case study also revealed that the foliar fungicides pyraclostrobin had the highest annual losses with erosion, thus increasing with corn stover removal levels (Figure 4). This was partly due to the fact that pyraclostrobin strongly adsorbs to soil particles as indicated by a high partitioning coefficient (K_{oc} = 11,000). This suggests that the magnitude of losses associated with varying levels of corn stover removal could potentially be greater on higher sloping soils that are highly erodible. As expected, based on a homogeneous crop-management system, pyraclostrobin losses were greater in southern and north central portions than in other parts of the state (Figure 5).

Key term

Corn stover: Stalks, leaves and cobs that remains in corn fields after the grain harvest

However, it would be expected that residue removal will not be a one-size-fits-all recommendation. This highlights another challenge in representing multiple land management options for regional model simulations using models such as GLEAMS-NAPRA. Surface residue removal has several trade-offs that need further investigation that considers crops best suited for specific regions. As an example, in colder climates excessive surface residue could reduce soil temperatures, delay soil drying during the spring and potentially delay spring planting. This could have tremendous implications on nitrogen and phosphorus mineralization as well as water quality.

▪ Policy implications

The production of biofeedstocks to meet RFS goals will result in significant modifications to landscapes in many locations of the USA. In other regions of the world, equally as significant or even greater modifications to the landscape will occur to address biofeedstock demands. These modifications will have impacts on both current and future policies. For example, within the USA, total maximum daily load (TMDL) analyses have been conducted for many watersheds. The introduction of significant biofeedstock production within these watersheds has the potential to greatly alter these TMDLs with biofeedstock production improving water quality in some cases, while potentially negatively impacting water quality in other instances. The introduction of biofeedstock production also has the potential to alter the selection and locations of best management practices within watersheds, which will impact numerous conservation programs at various levels of government ranging from local to national.

Government policies should consider the potential impacts of biofeedstock production on the environment and natural resources. Due to the complexity of biofeedstock-production systems and their interactions with watershed characteristics, potential impacts may not be readily identified. Therefore, hydrologic/water quality models will be important tools in assessing many of these impacts. Thus, enhancements to these models to accurately portray biofeedstock production, including establishment and harvest phases, will be critical. Biofeedstock production systems will likely alter ecosystem services and the ability to assess these impacts using models will also be important. Other public and private sector actions will also be necessary to insure the impacts of biofeedstock production can be fully and accurately assessed in a timely manner. Biofeedstock production may alter some areas quite rapidly and, thus, timely data on land use changes will be required. Remote sensing can be helpful in such instances in providing timely data. Runoff and water quality data from watersheds experiencing significant changes due to biofeedstock production will be important for ensuring models are able to capture impacts of biofeedstock production at watershed scales.

Future perspective

Data from plot-scale biofeedstock studies will continue to play an important role in providing data required for hydrologic/water quality modeling of biofeedstock production systems. Field- and watershed-scale studies will increasingly provide data to improve the ability of models to simulate the hydrologic/water quality impacts of biofeedstock production systems at these scales. One of the first watershed-level runoff and water-quality studies for a watershed with extensive switchgrass plantings has been initiated in Tennessee, USA.

The representation of common biofeedstock production systems within hydrologic/water-quality models will continue to improve. In particular, the establishment phases of biofeedstocks such as switchgrass and miscanthus will be sufficiently described to allow assessment of the environmental risks of biofeedstock establishment failure for a range of soil, climate and management conditions. The representation of biofeedstock harvest will also be enhanced so impacts to model parameters are described to reflect impacts on hydrology and water quality. Small plot and field data will provide much of the information required to greatly enhance descriptions of biofeedstocks in critical periods, such as during establishment and harvest.

Hydrologic/water-quality models will continue to evolve to represent the complexity of watersheds. The evolution of these models will allow them to increasingly represent the variability in watershed land uses introduced by biofeedstock production. The quantification of ecosystem services will become increasingly important and models that describe the hydrologic/water-quality impacts of biofeedstock production will be expanded or integrated with other models to describe the broader impacts of these production systems.

Decision-support systems will be created from hydrologic/water-quality models to assist stakeholders in quantifying the impacts of biofeedstock production and management decisions. These systems will utilize GIS and other databases to assist with applying a range of hydrologic/water-quality models to specific sites with site-specific management described to assist users in making improved decisions.

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Executive summary

- Hydrologic/water-quality impacts of various biofuel crop-production systems will be a function of feedstock of choice, watershed management and soil and climate conditions. Computer models can be used to efficiently evaluate various 'what if' scenarios related to biofuel crop production and their impacts on hydrology and water quality at various spatial and temporal scales.
- Primary limitations of the currently available computer simulation models include:
  - Insufficient data for calibration, validation and sensitivity analyses of the models;
  - Crop residue management and associated hydrologic/water-quality impacts representation in the models;
  - Inability to simulate various crop-management scenarios;
  - Inadequate representation of spatial and temporal processes;
  - Scaling up of results from plot scales to watershed and regional scales;
  - Need to quantify ecosystem services from various biofuel feedstocks;
  - Unavailability of easy to use decision support tools.
- These limitations need to be addressed before such models can be effectively used to make watershed management decisions for maximizing biofuel crop production and water-quality benefits.
- Water-quality impacts will vary under different climate, land use and soil conditions. Such impacts should be evaluated carefully so that appropriate management decisions can be taken to minimize any potentially adverse water-quality impacts.
- Development of easy-to-use decision-support tools that can be applied at various spatial scales (field scales to large watersheds) and inclusion of ecosystem service quantification, will greatly enhance the ability of the models to make sound watershed management decisions. We envision that the future model developments in the next 5–10 years will include these capabilities and will be widely used to evaluate impacts of various 'what if' scenarios on hydrology and water quality impacts of biofuel feedstocks.

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