Environmental Modelling and Software 108 (2018) 40–50

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

An integrated modeling framework for crop and biofuel systems using the DSSAT and GREET models

Ryan Anderson, Deepak Keshwani*, Ashu Guru, Haishun Yang, Suat Irmak, Jeyamkondan Subbiah

University of Nebraska-Lincoln, USA

ARTICLE INFO

Keywords:
Food-water-energy nexus
Crop modeling
Biofuels
Decision support system
Life cycle assessment
Service-oriented architecture

ABSTRACT

As global demand for food, energy, and water resources continues to increase, decision-makers in these sectors must find sustainable ways to produce and provide for the growing population. While many models have been created to aid in decision-making in these systems, there is a lack of robust integrated models that enable an understanding of the interconnections of these systems. This study develops a modeling framework that explores the connections of the corn and ethanol systems, two major food and energy resources. A crop modeling tool (DSSAT) and a biofuel life cycle assessment tool (GREET) are connected using a service-oriented architecture programming approach. A Python program is developed to connect these two models and run scenario analyses to assess environmental impacts of the integrated system. This paper explores the impact of decisions such as fertilizer use and plant population on environmental effects of greenhouse gases, energy use, and water in the integrated system.

1. Introduction

With the global population nearing 9 billion people by the year 2050, there is a need to better utilize the food, energy, and water (FEW) resources that are essential to living in the 21st century (Godfray et al., 2010). The population growth puts pressure on the existing resources which must be used more intelligently to support the projected population. The food and energy systems of the world are highly interconnected and understanding these interlinkages is vital in sustainably solving the resource demand problem that will perpetuate in the future (Bazilian et al., 2011). Energy is essential for producing crops, but with the progress of biofuels, food is also used as a means to produce energy which can displace the currently used fossil fuels. Crop modelers have been successful in modeling crop systems such as corn which can be processed into corn ethanol. Biofuel experts have also developed models for the biofuel system, but there is a gap in integrating these two systems using the existing tools. This is true for coupling any interconnected system in the FEW nexus.

Daher and Mohtar (2015) explore FEW modeling using a macroscopic approach. Their model, the WEF Nexus Tool, focuses on the environmental impacts of producing a certain food source of a whole region or country by estimating water, land, energy, and carbon requirements. The WEF Nexus tool calculates not only environmental impact, but also financial cost of either producing or importing the food source. Hang et al. (2016) on the other hand aims to integrate the FEW nexus on a local-scale rather than regional. It is also very general and can be applied to different food sources for a single production system. It uses an exergy balance approach to make calculations which gives the total environmental impact of the system using food, water, and energy.

Researchers have recently been attempting to couple systems to identify interlinkages in the FEW nexus. Some studies provide a general framework for systems of given scales and others aim specifically to connect certain agricultural systems. The International Food Policy Research Institute (IFPRI) developed the International Model for Policy Analysis of Agricultural Commodities and Trade (IMPACT) as a tool to understand the effect that certain policies and decisions have on sustainability and food security. IMPACT integrates economic, climate, and crop models to simulate the national and international agricultural markets. More meaningful assessments of the impacts on the environment, food production, and economy will result in including all system interconnections. (Robinson et al., 2015).

The Integrated Farm System Model (IFSM) is an example of an integrated model for specific agricultural systems as opposed to using general equations that can be applied broadly. IFSM integrates the crop and livestock systems to measure the total environmental impact of the decisions made in these sectors. The model requires inputs for eight

* Corresponding author. Department of Biological Systems Engineering, University of Nebraska-Lincoln, Lincoln, NE 68583-0726, USA.
E-mail address: dkeshwani2@unl.edu (D. Keshwani).

https://doi.org/10.1016/j.envsoft.2018.07.004
Received 21 December 2017; Received in revised form 6 June 2018; Accepted 5 July 2018
Available online 07 July 2018

different modules and modifies existing models to create a sustainability assessment (Rotz et al., 2012). The Biofuel Energy Systems Simulator (BESS) ties together the crop, beef, and ethanol systems. BESS calculates the production of each system and also provides a sustainability assessment over an annual production cycle (Liska et al., 2009). The CERES-Maize cropping model was integrated with the Root Zone Water Quality Model (RZWQM) to couple water quality with agricultural crop production. This was done to have a more comprehensive understanding of the interactions between these two systems as a decision support tool (Ma et al., 2006).

The MARKAL energy model and Center for Agricultural and Rural Development (CARD) market model were integrated to properly tie together the crop and biofuel systems. It is mainly an economic integration of two models that simulate the market for the biofuels. Their methodology involved linking relevant inputs and outputs of both models and analyzing the effect that certain events have on the market for fuels and related commodities (Elobeid et al., 2013). An environmental assessment of biofuel production in Greece was performed by using the GEMIS software as an LCA of biofuels from crop production to fuel and byproduct production. Four biofuel products were analyzed and compared based on environmental assessment results (Fontaras et al., 2012). Kim and Dale (2005) integrated several models and datasets to assess crop-biofuel system: DAYCENT for soil dynamics, NASS data for crop production and management, GREET for ethanol production, and the EPA-TRACI assessment method for environmental impact.

Validation is a concern for systems models because it is difficult to find empirical data to evaluate and improve the performance of the models using data measured in real-world environments. Tanure et al. (2015) developed a bioeconomic model focusing on the crop-livestock system by integrating validated equations and creating four sub-modules: herd structure and animal characteristics, animal nutrient requirements, weather-soil-pasture-animal integration, and economics. The individual equations used were pre-validated and then the whole model will be validated in a dynamic way by comparing scenarios to case studies of Brazilian systems of pasture-based beef cattle production. The IFSM has been slowly validating its simulations using data found in the Midwestern U.S., making it more accurate for temperate climates but less accurate for tropical climates (Tanure et al., 2015). Spatially integrated cropping models can be validated to the USDA NASS dataset. This is done by Zhang et al. (2010) as their Spatially Explicit Integrated Modeling Framework (SEIMF) data can be compared to geographic crop production data.

Previous attempts at integrated models were developed in the form of stand-alone software or programs. The individual systems are usually connected by writing the connecting formulas into a single program or running the models manually to develop assessments of the integrated system. This is seen in both the IFSM and BESS models as it integrates several systems using existing models by rewriting the equations as part of a new program. Since many individual models already exist in their own software, it would be much more practical to integrate them using service-oriented architecture (SOA).

SOA is a way to integrate software components as applications using communication subroutines. These models can be integrated as a web service and made available to users and developers as applications. This technique has been used for many disciplines to combine several systems together. The Open Geospatial Consortium (OGC) developed a Web Processing Service (WPS) to expose hydrological models as web services (Castronova et al., 2013). Users can use an Open Modeling Interface to predict runoff in certain areas by sending inputs to a hydrological model (TOPMODEL) which is available in a model workflow. Evapotranspiration calculation is another model that is required in the workflow and an example of integrated models working together on a web service. Many researchers have used web services and SOA to couple climatic and hydrological models to understand the integration of these two systems or for specific end user application such as flood emergency response (Goodall et al., 2011, 2013; Tan et al., 2016).

In the field of bioinformatics, the European Bioinformatics Institute (EMBI) developed a loosely coupled web service that allows users to access large databases, search tools, and analysis tools (McWilliam et al., 2013). Analysis tools such as genetic sequence similarity and biological sequence alignment are integrated via advanced workflows with available data in the data repository. Users can integrate additional functionality to web sites and programs on the web. For social sciences, several web services exist to analyze the sentiment and opinions of the public for various online services such as Youtube, Twitter, and Facebook (Serrano-Guerrero et al., 2015). These analysis tools are models that are exposed as a web service application and can analyze data for companies to incorporate into their software. The models are integrated into a workflow and can be used by developers to build analytical tools.

Agricultural models have not capitalized on SOA to improve decision making and to couple systems, including the crop and biofuel systems. With a loose coupling framework, these models can be available for anyone to use independently with their original functionality, but can also be used together to run crucial impact assessments. More specifically, the tool developed through this study will help crop growers and biofuel producers intuitively utilize these models together to understand how different decisions they make can affect the environment on a larger system boundary. This will make computation of the environmental impact more practical. The SOA can be created as a web-service that any user is free to use either to write their own software or to call the functions directly.

The objectives of this study were to:

1) Develop a framework for integrating two well-accepted, validated models in the cropping and biofuel systems using a service-oriented architecture
2) Evaluate scenarios to demonstrate the utility of the framework as a decision support tool
3) Conduct a sensitivity analysis to determine effects of varying key model parameters on system response.

2. Material and methods

2.1. Model description

2.1.1. Model identification

Desirable attributes for models are wide acceptance, high validity, and high functionality. The cropping models need to take weather, soil, and management inputs and output potential yield for that season. The biofuel model must take crop yield and key resources in production (i.e. fertilizer, irrigation) to output not only fuel production but also environmental impacts of resource use and emissions. There exist several models that simulate the crop and ethanol systems individually. Because the crop system is inherent to biofuel production, they must be coupled in order to understand the interactions between the systems.

de Carvalho Lopes and Steidle Neto (2011) break down many of the cropping models that are widely used and validated in their respective fields. Some of these models include CERES, CROPGRO, Environmental Policy Integrated Climate Model (EPIC), Hybrid-Maize and APSIM. Additionally, the Decision Support System for Agrotechnology Transfer (DSSAT) is a program that acts as a wrapper function for many different cropping models, including the popular CERES and CROPGRO (Hoogenboom et al., 2015). All tools successfully model the cropping system of interest and are meant to be used as decision support systems for either private decision makers or policy makers. The spatial and temporal scales and equations may differ from model to model, but the functionalities are similar.

DSSAT is used in more than 100 countries and has been under constant development for more than 20 years. DSSAT also has a high volume of data backing up calibrating its models so it can be used to predict crop yield in a variety of locations with high validity. There are over 60 inputs that can be plugged into the DSSAT model which shows how functional it can be for researchers and if the model can be properly wrapped, DSSAT can offer high functionality into the integration of the crop and biofuel systems.

DSSAT has also been integrated with other models in the past. The IMPACT model, for example, integrates DSSAT for their crop production module when determining the potential for food supply. IFSM uses equations found in DSSAT to calculate their crop yields. DSSAT is not only high in functionality, but researchers have experience in integrating it with other systems as well, making this the best tool to use for our application.

Since biofuel production is closely associated with environmental impact, most of these models are life cycle assessments (LCA) in order to determine the environmental effect/benefit of producing a certain type of fuel from raw materials to consumption. Some well-known fuels LCAs include the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) Model, SimaPro, the Global Emission Model for Integrated Systems (GEMIS), and the MARKet ALlocation model (MARKAL). The GREET model is widely used, largely because it is sponsored by the US Department of Energy (Elgowainy et al., 2012) and Argonne National Laboratory consistently updates the data that drives the model. The latest major update to the corn ethanol pathway was in 2014 and the current GREET version used is GREET 2015 (Wang et al., 2014). When performing LCA with GREET, it includes the crop farming pathways, which give some functionality to the user in defining cropping inputs. For example, the corn ethanol pathway includes the corn farming process, which allows the user to specify irrigation, fertilizer, and chemicals per unit weight of corn produced. The MARKAL model behaves in a similar way to calculate environmental impact of biofuel production with a large database. It also includes a linear programming algorithm that helps the user in determining the least-cost solution on the energy resources to use (Kannan et al., 2007). The purpose for this model however is not to find an optimal solution for the user but to calculate the system impact from decisions defined by the user. MARKAL also does not have near the user base or support that GREET has. Given its numerous benefits, GREET is the chosen biofuels model.

DSSAT and GREET are also capable of simulating a wide range of different crops and biofuels. This study will focus on integrating the corn and ethanol systems, but the same principles can be applied to a variety of biofuel systems such as biodiesel from soybean or ethanol from corn residue.

2.1.2. Computational structure

The SOA will follow the framework described in Fig. 1. The middle layer shows the model pipeline and at the very bottom are classes that create inputs from user actions. These feed into the Control and Batch methods that create the crop experiment file and batch file for the DSSAT model under the DSSATFile class. DSSATFile is inherited by the DSSATModel class which runs the file created from the user inputs. DSSATModel returns yield and all other outputs associated with DSSAT. This is inherited by the DS_GREET class which runs the GREET model biofuel pathway based on the crop outputs simulated by DSSAT. Every module of this structure can be called by a client on a Representation State Transfer (REST) server. Any user that has access to the server can make requests to the server to utilize the integrated model in the middle layer. The integrated model interacts with a data repository to store and access data that are used in the subroutines.

2.1.3. DSSAT wrapper

The cropping model in this integrated model should be able to simulate crop yield based on several environmental factors and management practices that the user controls. Creating a wrapper for the DSSAT model allows the program to run and be connected to other programs, which makes it viable for integration. pyDSSAT is a Python wrapper that runs the DSSAT model in its original FORTRAN code (He et al., 2015). The program makes a large number of input assumptions and also wraps the model by compiling the original FORTRAN source code. The program is open source so it was used as a reference to write the Python code used in our wrapper.

The method for writing the DSSAT wrapper follows a similar flow to pyDSSAT and is shown in Fig. 1. It must create an experiment file based on farming inputs, run the file through the model, and process the outputs. The experiment file used by DSSAT is a text file that compiles the inputs in a certain format for the simulation that the user wants to run. In our implementation, this is created by making a Python class, DSSATFile. The pyDSSAT code allows the user to input the following variables: crop type, soil type, weather station, start year, end year, planting date, and model mode. The integrated model only simulates one year, so end year is not needed. It is also only being run in batch mode where a single experiment file is being used so the mode is defaulted as "B" for "Batch". Since DSSAT is robust and has many inputs, it is difficult to fit them all as inputs into one class practically. Other classes were created to enter management data as comma separated files (CSV) files. Irrigation, fertilizer, harvest, tillage, and chemical application all have their own class defined to take in scheduling inputs written to a CSV file.

The DSSAT model can be run in the command line using DSCSM046.exe which is available with installation of the software. pyDSSAT runs the model by compiling Fortran code but running the batch file in the command line is simpler and provides the same results. The pyDSSSAT class, DSSATModel, runs the model by calling the executable in the terminal and taking in data from the experiment file and the management files. The model controller finishes writing the experiment file that did not yet include the management inputs from the irrigation, fertilizer, harvest, tillage, and chemical classes. After the model is run, it creates output files that show results for yield, crop growth, soil-water balance and more.

2.1.4. GREET wrapper

The objective of the biofuel model is to not only calculate the total biofuel production from crop production, but also the resource use and emissions associated with the biofuel in comparison to a reference fuel. To understand the environmental impact of producing the clean burning fuel, the biofuel pathway is compared to the reformulated gasoline pathway. GREET can compare LCAs of different fuels such as ethanol and gasoline on a per MJ basis. The pathways in the GREET model used for this tool are the "E85 Gasoline Blending and Transportation to Refueling Station" pathway and the "Reformulated Gasoline (E10) Blending and Transportation to Refueling Station" pathway.

The ethanol pathway is broken down into several processes and calculates all results associated with this pathway. It begins with the Corn Production for Biofuel Refinery process which includes some inputs and outputs found in DSSAT. This is where the DSSAT inputs are written into the GREET model when appropriate. The results feed into the ethanol production process which is chosen as "Dry Mill Ethanol Production w/Corn Oil Extraction" since this is a common method in many ethanol plants in the U.S. While the user can specify the percent of ethanol being produced from each process in the software, for this study, it was assumed that 100% of the ethanol produced is from dry mill with oil extraction. GREET calculates emissions from the beginning of the corn farming process to the end of the transportation process to show final resource results for the pathway.

While many inputs in GREET overlap with DSSAT inputs, others are more difficult to estimate. The rest of the inputs require the user to know how energy and resources as a whole are used for the rest of the operations such as vehicle usage, tillage, and transportation. GREET also has numerous libraries and pathways for resources that can be edited. The defaults for these inputs are US averages so for the purposes of this study, the default energy uses were kept to make the tool more

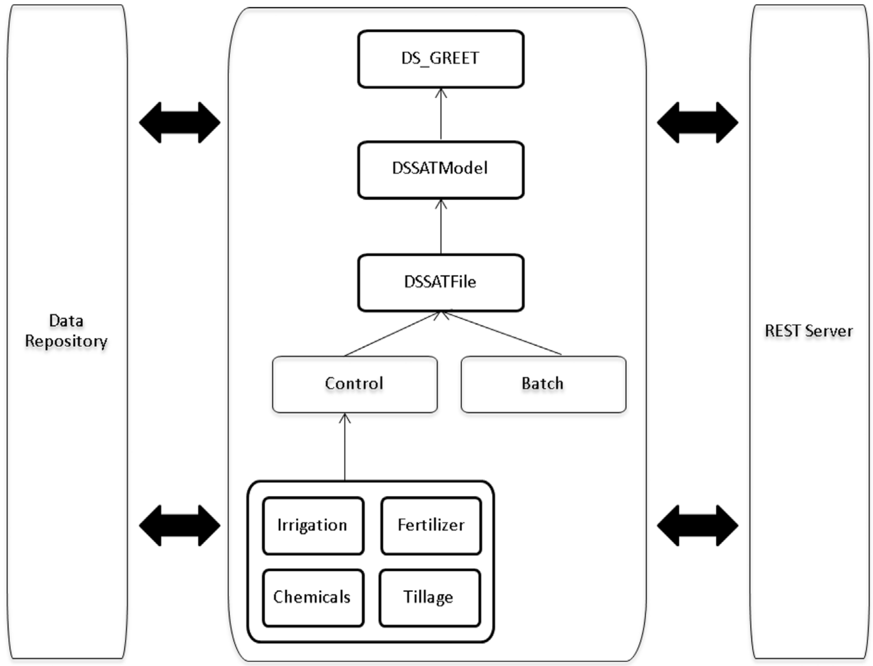

Fig. 1. Computational model pipeline.

intuitive.

GREET uses terminology called Well-to-Pump (WTP) and Pump-to-Wheel (PTW) to describe where the product is in its life cycle. The WTP pathway describes resource use and emissions associated with the production of a product from its raw materials to transporting it to a fuel pump ready to be consumed. The PTW pathway describes resource use and emissions associated with the consumption of the product. This study will look at the full Well-to-Wheel (WTW) pathway of the corn ethanol lifecycle.

The corn ethanol pathway in GREET uses a displacement method by default, and Distillers Grains and Solubles (DGS) displaces animal feeds which is a mix of corn, soybean meal, urea, and soyoil for different types of livestock. The displacement values per feed and livestock are averaged and used as the allocation amount to credit to DGS byproduct. Because of the displacement of soybean meal and soybean oil, the water consumption associated with them is taken as credit, which may result in a negative WTP water consumption value if irrigation amount is too low. This must be considered when making conclusions from the GREET results. Also, while DSSAT calculates some environmental footprints such as water use for corn, GREET already takes into account the footprint produced from corn farming. Hence, any environmental assessment done in the integrated model is done based on GREET values, not DSSAT.

GREET operates based on calculating environmental results from ethanol amount, but the DSSAT model only provides corn yield. The program must convert kg/ha of corn to total liters (L) of ethanol based on GREET's current conversion rate of 10.598 L ethanol/bushel corn. Since a liter of E85 does not provide the same amount of energy as a liter of E10, the volume calculated must be converted into energy (MJ). Further, the crop farming inputs in GREET are on a per unit weight of crop produced basis while the user inputs these values on a per hectare of field basis in DSSAT. Irrigation and fertilizer inputs from DSSAT are converted accordingly to be written into the.greet file.

CalculatorBatch is a program that was compiled using an API developed by the makers of GREET. The arguments for this program are the.greet file name, year(s) of simulation, and the ID for the fuel pathways or mixes. The GREET wrapper runs the written.greet file into the CalculatorBatch program using the values specified by the farming system. There are two pathways being used – Corn Ethanol Production and E10 Reformulated Gasoline – so the GREET model is ran for both pathways using the amount of energy produced in ethanol production.

While this API is a useful tool and essential for the development of this wrapper, it is only able to calculate resources for WTP and does not include the results from actual usage of the fuel. Much of the offset in emissions and resource use comes from the burning of the biofuel in comparison to fossil fuel so it is essential to include the PTW pathways as well. Fortunately, only the WTP pathway results are variable due to the cropping inputs of irrigation, fertilizer, and chemicals. The PTW results do not change on a per MJ basis since those are completely separate from production and only dependent on the vehicle that is consuming the fuel. The results for these PTW pathways on a per MJ basis were stored in a separate class wherever there were PTW emissions present. Once the total amount of ethanol energy is calculated from the beginning of the program, it is input into the PTW class to output total resources. The vehicles chosen for both pathways were ones that are commonly found for their respective fuels; Flex Fuel Vehicle (FFV) was used for ethanol while Standard Ignition Internal Combustion Engine Vehicle (SI ICEV) was used for E10 Reformulated Gasoline. Flex Fuel Vehicles have engines that are able to burn fuels that have higher blends of ethanol which is why they are commonly used for E85 (Alternative Fuels Data Center, 2017). E10 gasoline is similar enough to gasoline that a standard internal combustion engine found in most vehicles can run it (Anjikar et al., 2017). After adding results from the API along with results from the PTW class, the program will output total (WTW) results for ethanol and gasoline. The total flow of the program from inputs to outputs is represented in Fig. 2.

2.2. Post-processing

The design for post-processing the resource results is based on Wu et al. (2007) who evaluated the benefits of using ethanol relative to gasoline for fueling vehicles. The main outputs that this study analyzes are greenhouse gas (GHG) emissions, energy usage, air pollutants, and water consumption. GHG emissions are calculated as CO_2 equivalent from CO_2, CH_4, N_2O, and biogenic CO_2 based on their global warming potential values (1, 25, 296, and 1 respectively) (IPCC, 2007). The criteria air pollutants identified when comparing the two fuel pathways are Volatile Organic Compounds (VOC), CO, Nitrous Oxide (NOx),

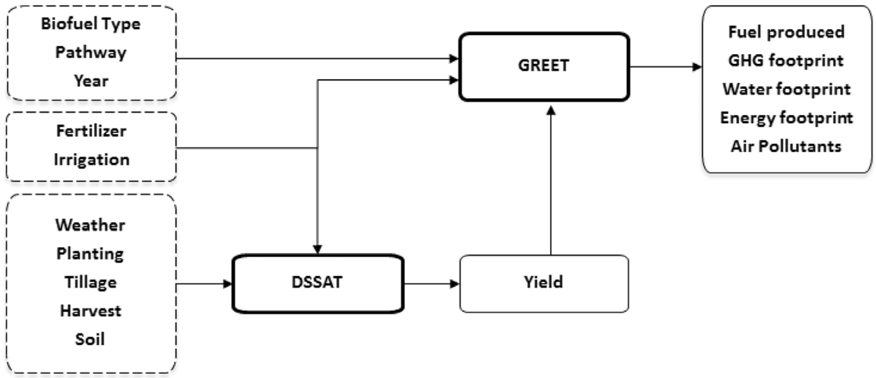

Fig. 2. Flow diagram of DSSAT-GREET model connections in Python program.

Particulate Matter (PM10), and Sulfur Oxide (SOx). These are all significant emissions produced in the corn ethanol pathway that affect human health. The energy savings from nonrenewable fuel use are also important to analyze as total fossil fuel energy and petroleum fuel energy use are compared in this model. Fossil fuel energy consists of total use from coal, natural gas, and petroleum energy in the life cycle. Petroleum fuel use is singled out from the other fossil fuels because most of the benefit from producing ethanol comes from the reduction of petroleum fuel. Water consumption is highly sensitive to irrigation in the crop pathway and can be beneficial or detrimental based on management and weather.

After the yield is calculated in DSSAT in kg/ha, it is converted to ethanol in MJ. To compare the ethanol production to gasoline, an equivalent amount of MJ of gasoline is calculated in the GREET life cycle and the two pathways are compared to each other. In this study, the functional unit of comparison is total MJ of E85 possibly produced by 1 ha of corn production. This effectively defines the system boundary to start with production of cropping inputs and end with the consumption of E85 fuel in a vehicle. The LCA tracks fertilizer and chemical inputs down to energy inputs of raw materials such as ammonia and phosphate. Environmental footprint of raw materials for ethanol production are tracked for enzymes, yeast, and chemicals. Blending gasoline for E85 is also tracked along with its raw inputs. The system boundary ends once the fuel reaches the vehicle that uses it and is consumed. Since DGS displacement of livestock feeds is credited, the boundary also includes consumption of DGS and its environmental benefits.

There are two ways to compare the footprint of E85 fuel to E10 fuel: one is by total footprint and the other is percentage footprint of E10. Simply subtracting the results from the E85 gasoline pathway from the E10 pathway provides the absolute savings. Percentage savings is the percent of the resource saved by using E85 as opposed to E10. This provides a normalized value that can be compared across different categories. Negative values for either method show that producing ethanol is beneficial to gasoline in that category. Wu et al. (2007) used percentage savings to compare several different fuel pathways on a per unit of distance basis. It is important to understand both methods when making the assessment since absolute savings encourage larger crop and biofuel production operations while percentage savings encourage more efficient operations on a per unit of energy basis. This gives the user more options on how they can make operations decisions that may be more environmentally sound.

As an additional note, 'water footprint' is commonly used referred to as a way to track the use of water in different phases and stages of a process. In this paper, 'water footprint' is defined as the difference in total water consumption between E85 and E10 life cycles. A framework for water tracking was not included for this paper in the GREET model.

2.3. Scenario analysis

2.3.1. Base scenario for comparison

The driving inputs of both models are nitrogen amount from fertilizer application and water use from irrigation. This is because these management inputs have a high effect on yield depending on the growing conditions, and have a high environmental footprint from life cycle production and use. A sensitivity analysis of the effect of fertilizer on the integrated model was conducted to determine the impact on the system from changing one of the parameters.

A base scenario for corn production is developed from regional data and management recommendations of corn farming in the Eastern Nebraska region. This scenario is based only on environmental and user inputs as GREET default values for emissions and energy use are kept the same. The sample field location and year used are Mead, NE, and 2015. Weather data for this season were obtained from the High Plains Regional Council Center (HRPCC) in the form of daily precipitation, minimum temperature, maximum temperature, relative humidity, solar radiation, and location coordinates. The plant population for irrigated corn that is typically used in the Midwestern region is approximately 10 plants/m^2 (Barr et al., 2013). Anhydrous ammonia is a common fertilizer material used for nitrogen application so this method was used for the baseline scenario. The corn hybrid chosen for this study, called "GDD2600", has a 113-day maturity (medium season hybrid) from planting to physiological maturity. The soil type used should accurately reflect the profile found in Eastern Nebraska corn fields so the soil file in DSSAT chosen is for loamy soil. This soil file gives descriptions by layer based on water holding capacity, density, and nutrient characteristics. The water holding capacities were adjusted based on local data to more accurately reflect the Nebraska soil profile (unpublished research data). Values for Field Capacity (FC), Wilting Point, and Organic Carbon Matter (OMC) are represented in Table 1.

Planting and harvesting dates are based on data from the USDA National Agricultural Statistics Service (NASS). In Eastern Nebraska, recommended times to plant corn are between April 27th and May 18th while the recommended times to harvest corn are between October 4th and November 10th (USDA, 2010). Thus, the dates chosen for planting and harvesting are May 1st and October 15th respectively. Fertilizer

Table 1
Soil values by depth.

Soil variable	0–30 cm	30–60 cm	60–90 cm	90–120 cm
FC (% vol)	35.4	30.0	29.8	32.0
PWP (% vol)	23.0	18.6	18.8	19.4
Sand (%)	35.1	37.5	34.4	29.6
Silt (%)	48.6	43.2	40.9	42.7
Clay (%)	16.3	19.3	24.6	27.6
OMC (%)	3.5	2.7	2.0	1.6

Table 2
Values for baseline corn production scenario.

Parameter	Baseline Value
Location	Mead, NE
Year	2015
Plant population	10 plants/m^2
Fertilizer material	Anhydrous ammonia
Fertilizer amount	150 kg N/ha
Fertilizer application method	Banded on surface
Soil	Silty Loam
Planting Date	May 1
Harvest Date	October 15
Cultivar (Hybrid)	GDD2600
Irrigation Management	Automatic when needed
Irrigation application method	Sprinkler
Row spacing	75 cm
Plant depth	5 cm
Tillage method	Drill, no-till

amounts used in the simulations were based on the amounts used in long-term field research conducted by Irmak (2015a; 2015b). In Nebraska, it is common to apply fertilizer using side-dressing and especially since it is being applied on the same day as planting, it is used for this scenario. In DSSAT, this application method is named "Banded on surface". Phosphorous and potassium are normally not included in fertilizer for corn so these were left out of the simulation. DSSAT has an option to automatically irrigate the field if it senses water stress throughout the season. Water stress for yield should not be a constraint for this simulation so irrigation was simulated using automated irrigation option so that water is not a constraint for achieving potential grain yield. The state of Nebraska has a large aquifer and uses groundwater for irrigation. Nebraska commonly uses center pivots to irrigate their fields so the equivalent setting in DSSAT was set to "Sprinkler". All baseline values are recorded in Table 2.

Pesticide use is an option for this integrated model but was left out of this case study since DSSAT does not handle pest hazards well when predicting yield. If pesticide use were to be included, the integrated model would only calculate the negative environmental impacts from GREET and leave out the positive yield effects it has on cropping. In this scenario, it is assumed that there are optimal conditions for pests and weeds so pesticide chemicals are not used. Tillage settings are also important to consider in this integrated system and in DSSAT, it is defined as "Drill, no-till". This is not defined in GREET however due to the difficulty of adding vehicle fuel use in the tool.

2.3.2. Nitrogen fertilizer sensitivity

The production of corn has several sources of emissions such as soil emissions, fuel use, and chemical applications. The corn production process in GREET has default values of 2.40 g/bu (0.095 g/kg) and 2.73 g/bu (0.107 g/kg) of NOx and N2O emissions respectively due to soil and fuel use. Fertilizer applications have high added environmental impact and increase the LCA for corn ethanol's emissions. Nitrogen amount was analyzed relative to the baseline value of 150 kg N/ha which is normal for this field. The following values for nitrogen application were run in the model assuming the baseline scenario for all other variables: 0, 50, 100, 150, 200, 250, and 300 kg N/ha. Resource savings from producing E85 over E10 were calculated both as a total difference and as a percent reduction. Total footprint shows the physical results and changes with each scenario while percent footprint shows the sensitivity of output parameters to nitrogen fertilizer application.

The pathway is separated into WTP and PTW which both have different contributions to the overall results. To quantify the difference, the program was altered to calculate emissions from WTP and PTW separately. The two results of GHG emissions and nonrenewable energy use were compared to each other based on these different pathways.

Table 3
Nitrogen values for each plant population scenario.

Plant pop (m^{-2})	Nitrogen (kg N/ha)	Yield (kg/ha)
5	90	9802
6	110	10679
7	110	11048
8	120	11498
9	120	11849
10	120	11967
11	120	12146
12	130	12556

2.3.3. Optimal plant population

A range of plant populations was used to gauge the sensitivity of this input on the DSSAT model. There are significant breaks in the relationship between plant population and yield for values under 40k plants/ha and over 120k plants/ha so this sets the bounds for values of plant population (Table 3). Therefore, the model was run for plant populations in the range of 5–12 plants/m^2 over the span of 15 years from 2001 to 2015. This will show the relationship between varying weather and the optimal plant population as a possible decision point for farmers. With higher plant population, in general, higher nutrient application is required. Each plant population was run with a range of nitrogen fertilizer amounts to determine the optimal value. Nitrogen fertilizer values from 10 to 600 kg N/ha were used to show the full relationship of nitrogen to yield for this plant population and the maximum described by DSSAT. The optimal nitrogen application amount was determined by picking the value where yield exceeds 90% of the max as shown in Fig. 3. This was done to ensure that a consistent fertilizer value was chosen for each plant population depending on the nutrient requirements.

Once nitrogen amounts are picked for each plant population, they were used as input into the model to calculate resource results for each scenario. Since nitrogen amount increases with plant population, the results should reflect an increase in GHG footprint. However, if the yield gains offsets the nitrogen use, then the GHG footprint can actually be reduced.

To show the complete GHG footprint matrix in relation to plant population and nitrogen fertilizer application, combinations of both variables were run. Plant populations were inputted in the range of 5–12 plants/m^2 and nitrogen applications were inputted in the range of 100–250 kg N/ha with increments of 1 plants/m^2 for plant population and 10 kg N/ha for nitrogen applications. The GHG footprints of each scenario are calculated to show the relationships with both of these

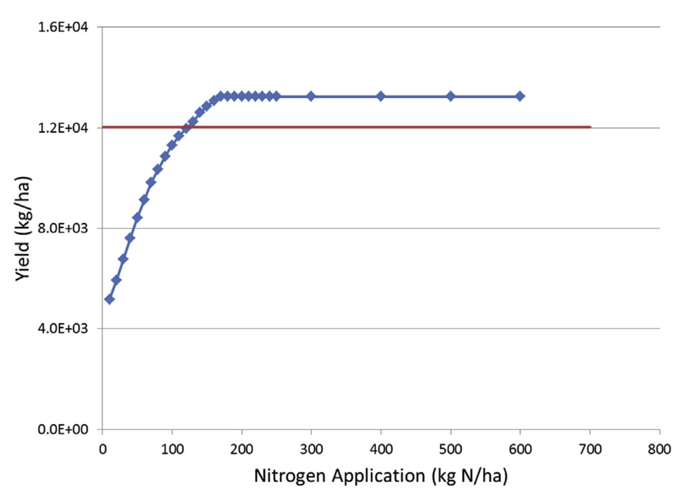

Fig. 3. Nitrogen application vs yield of plant population of 10k plants/ha. The horizontal line represents 90% of max yield. The nitrogen amount chosen for 10k plants/ha is 120 kg/ha.

variables simultaneously.

3. Results and discussion

3.1. Model verification

Before performing analyses, the Python program must be verified with the models in the original software. Verification of the DSSAT wrapper is done by running the model twice using the same scenario both manually through the DSSAT software and with the InputCreator class in the wrapper. Both programs produce a summary file that shows generic outputs of the simulation run including yield, seasonal weather data, soil water balance, and management summary. Three scenarios with three different nitrogen fertilizer amounts (0, 100, and 200 kg/ha) were run in both programs and the summary files exactly matched which verifies the accuracy of the wrapper.

Verification on the GREET model is done in a similar way by running the software manually using a scenario and then running the same scenario with the GREET wrapper written in Python. The WTP pathway is run with the wrapper so that part is validated with the software. The results in the wrapper are based on total emissions from the amount of energy produced in DSSAT since it is inherited so the scenario that is run manually through GREET must be done on the basis of total energy produced. The same baseline scenario is run through the program to get results from the GREET model. Only the WTP results are printed to compare to the results obtained from manual use of the model. PTW calculations are linear and directly taken from the model so these do not need to be verified.

The comparisons are shown in Table 4 where results are calculated on the basis of the amount of energy created from the ethanol process. The error between the two results is minimal and is attributed to rounding error from the GREET software.

3.2. Sensitivity and scenario analysis

3.2.1. Sensitivity analysis on nitrogen fertilizer

Fig. 4a and b shows the results for nitrogen application on GHG emissions and nonrenewable energy use overlaid with the corresponding yield. Up to 100 kg N/ha, increasing nitrogen application increases the yield potential and lowers the GHG footprint of the system since more E85 energy can be produced to displace E10. However, yield levels off after this value and can no longer offset the footprint caused by increasing nitrogen rate. Therefore, the GHG footprint of the system will sharply increase beyond 100 kg/ha because these emissions are highly sensitive to nitrogen fertilizer use as displayed in Fig. 4a.

The total footprint of both nonrenewable energy categories in Fig. 4b shows a steady increase that evens out past 150 kg N applied per hectare. Fossil fuel and petroleum fuel footprints appear to closely mirror the relationship between yield and nitrogen rate. This means that these footprint categories are more sensitive to the amount of E85 produced than the amount of nitrogen applied. The petroleum fuel footprint is the lowest as E10 requires much more petroleum in production than E85 on a per MJ basis. The total fossil fuel footprint is not as low because E85 is detrimental (higher footprint) in comparison to E10 in its coal and natural gas footprint. Fig. 4b shows this as the petroleum fuel continues to steadily decrease with nitrogen application while the total fossil fuel footprint starts to increase as yield levels off.

The sensitivity is more clearly shown in Fig. 4c that normalized footprint for each category in comparison to the optimal fertilizer rate according to GHG footprint. The trends look different in this subfigure because it is comparing all scenarios to a central value of 150 kg N/ha.

Table 4
Verification of wrapper program with GREET software for items per hectare.

Categories	Wrapper	Software	% Error
Fossil Fuel (MJ)	65878.11	65410	0.72
Petroleum Fuel (MJ)	26818.86	26375	1.68
VOC (g)	4356.1	4360	0.09
CO (g)	3037.1	3040	0.10
NOx (g)	7065.3	7070	0.07
PM10 (g)	1109.1	1110	0.08
SOx (g)	4302.2	4300	0.05
CH4 (g)	12385.9	12390	0.03
N2O (g)	2446.9	2450	0.13
CO2 (g)	3365647.8	3365090	0.02
CO2_Biogenic (g)	−582.6	−580	0.45

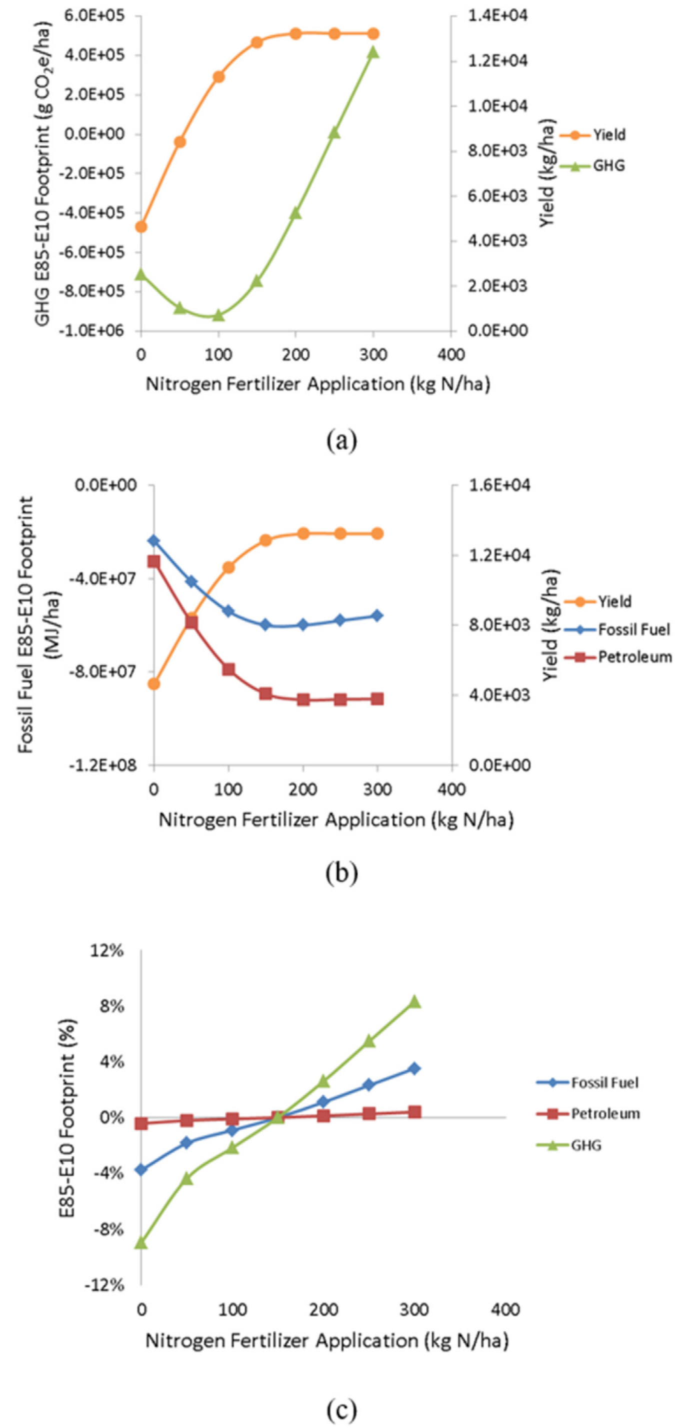

Fig. 4. E85-E10 total footprint of (a) GHG emissions and (b) fossil fuel energy balance and (c) percent footprint of all categories in comparison to middle of 150 kg N/ha.

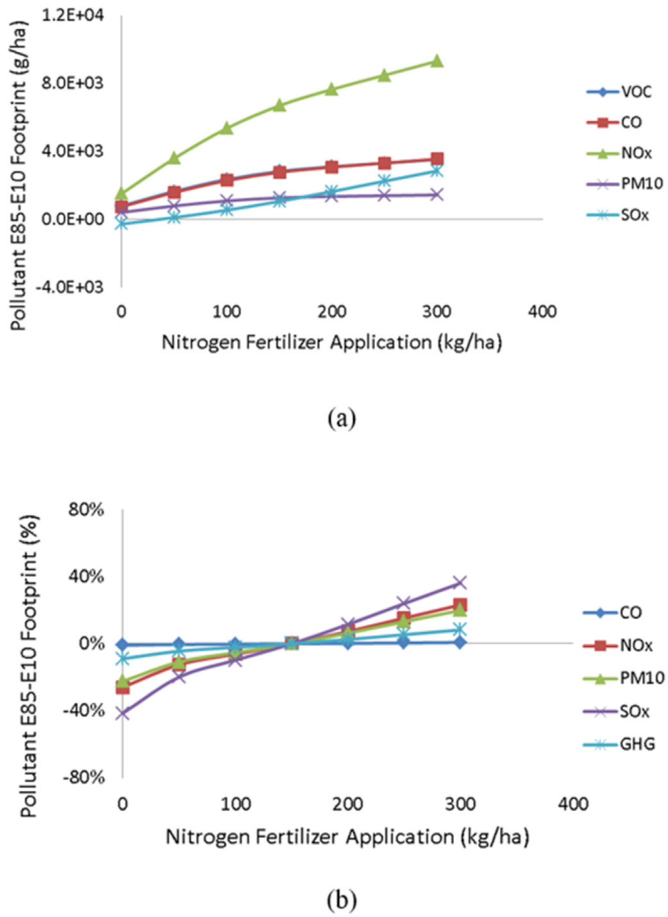

Fig. 5. E85-E10 criteria pollutants (a) total footprint and (b) percent footprint as compared to optimum of 150 kg N/ha of fertilizer application.

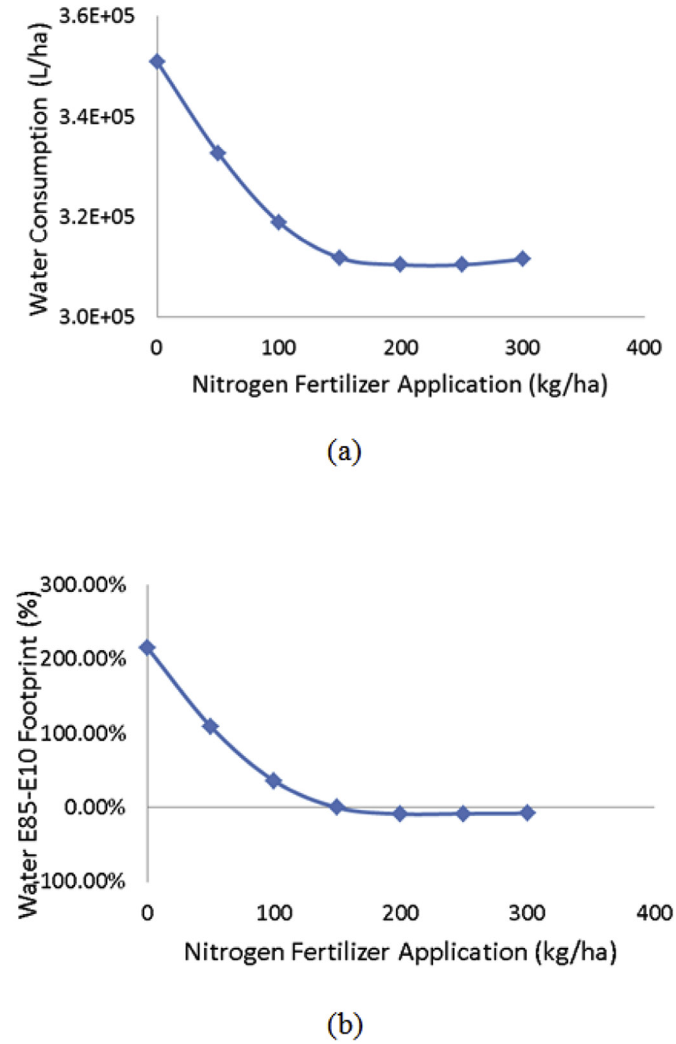

Fig. 6. (a) E85 total water consumption and (b) E85-E10 percent footprint compared to optimum of 150 kg N/ha.

The percent change in footprint is much higher for GHG across the range of nitrogen rates in comparison to the fossil fuel categories. Petroleum fuel also shows very little sensitivity to nitrogen which confirms the findings from Fig. 4b. This integrated model can inform decision makers on the optimal fertilizer application not only based on yield but based on environmental impact. In the model, yield would continue to increase with increasing nitrogen but with GHG savings, there is a clear optimum value for this scenario at 100 kg N/ha.

While E85 is beneficial to E10 for all of the categories described above, it is not as beneficial in emission of criteria pollutants as found in Fig. 5. In every scenario and for each category, E10 gasoline emits fewer pollutants than E85. With increasing nitrogen application, the emissions footprints become more positive. This shows one of the tradeoffs of producing ethanol when using it to displace reformulated gasoline as a fuel. Each pollutant shows a similar increasing trend in Fig. 5b where emissions compared to the middle nitrogen scenario of 150 kg N/ha. NOx emissions are impacted the greatest with increasing nitrogen which is reflected in GREET's Nitrogen and Corn Production pathway. In the Nitrogen mix pathway, producing 1 kg of nitrogen emits 7.46g NOx and in the Corn pathway, 1bu of corn emits 2.40g NOx.

Water consumption in the crop-biofuel system is influenced by irrigation amount and the amount of water used in the ethanol plant for producing ethanol. Processing water consumption for ethanol is greater than gasoline marginally by about 0.076 L/MJ. However, irrigation has the most significant impact and the practices that a decision maker has can greatly influence the water footprint of corn ethanol. In this scenario, irrigation is automated when needed. If the crops grow larger due to increased nitrogen, then more irrigation may be needed to maintain the growth and should reflect larger consumptive use. Fig. 6a shows the total water consumption from the E85 pathway in relation to nitrogen application rate. Water consumption has a negative trend with nitrogen, even though yields are increasing and consumption is expected to rise. The results indicate that DSSAT may not be able to properly handle the relationship between nitrogen and water consumption. Climatic conditions influence how increased nitrogen levels impact crop physiology, yield, and evapotranspiration which is not a linear response. In this scenario, the annual precipitation is 731 mm which is high for this region. The percent footprint though does show a clear downward trend of water footprint with higher fertilizer. The increase in yield creates a lower water footprint and offsets the use from irrigation which does not change as much.

Fig. 7 shows the breakdown of the footprints between the WTP pathway and the PTW pathway for GHG and fossil fuel categories. The production of ethanol emits more CO_2e than gasoline on a per MJ basis and that is reflected in the WTP results where emissions increase as nitrogen use increases. Conversely, the GHG emissions for the PTW pathway decrease due to consumption of ethanol as E85 use emits much less GHG's than E10 and offsets the GHG increase from the WTP pathway as seen in the full WTW pathway. The footprint is negative through this range of nitrogen application but as it gets higher, the PTW footprint levels off and WTP footprint continues to increase at a near-constant rate. The total WTW pathway shows a net negative footprint for ethanol which shows the offsetting effects of clean consumption in

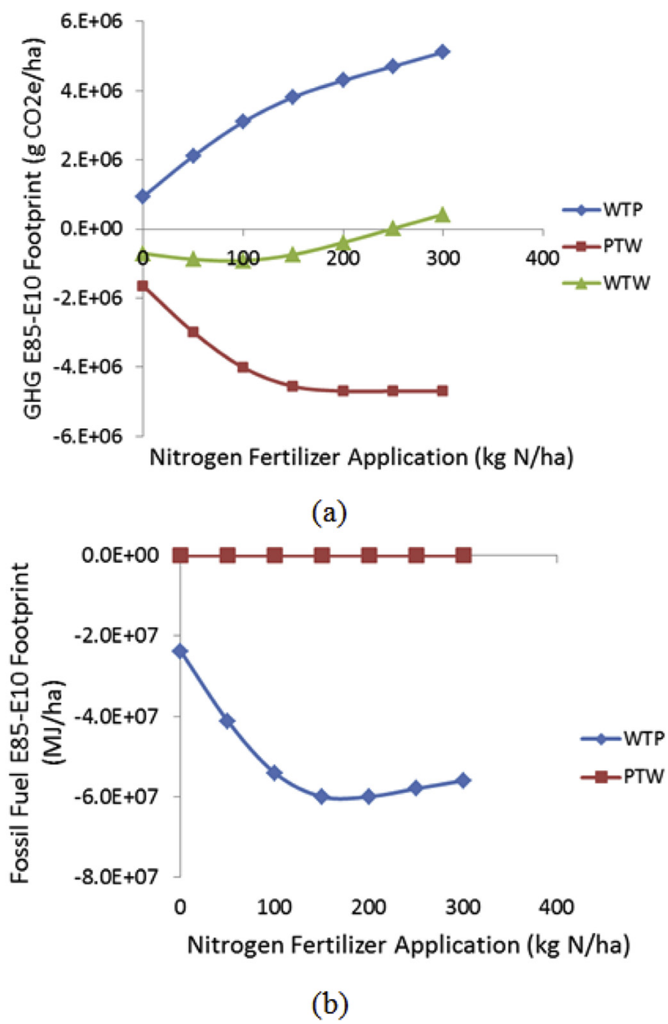

Fig. 7. Comparison of Well to Pump (WTP) pathway in E85 footprint to Pump to Wheel (PTW) pathway for (a) GHG emissions in a wet year and (b) fossil fuel use.

vehicles.

PTW footprint does not have an impact on any of the other categories. The differences between E85 and E10 come only from the WTP pathway in all of these resources. This is because in the WTW analysis, the vehicle used for both E85 and E10 fuels are kept the same. Since the engine that is burning the fuel is standardized, there is no difference in energy, water, or air pollutant savings per MJ of E85 and E10. For example, Fig. 7b shows that fossil fuel footprint only changes with the production of the fuel, not the consumption. GHG emissions is the only category where there is a difference between E85 or E10 consumption because of the composition of the fuel.

3.2.2. *Optimal plant population*

Fig. 8 shows the relationship between total resource and emissions footprint and plant population. The fossil fuel energy footprint steadily decreases with increase in plant population. This is because, based on the assumptions made within the DSSAT model, the increasing nitrogen application does not have as much of an offsetting effect on the energy footprint from producing with a higher plant population. GHG emissions footprint on the other hand is heavily influenced by nitrogen application and that shows in Fig. 8a where it steadily increases. The GHG footprint levels off after 9 plants/m^2 because nitrogen levels are also leveling off as shown in Table 3. Much like in Section 3.1.1, the criteria pollutant footprints increase with plant population and are a net positive compared to using E10 gasoline. With this scenario analysis,

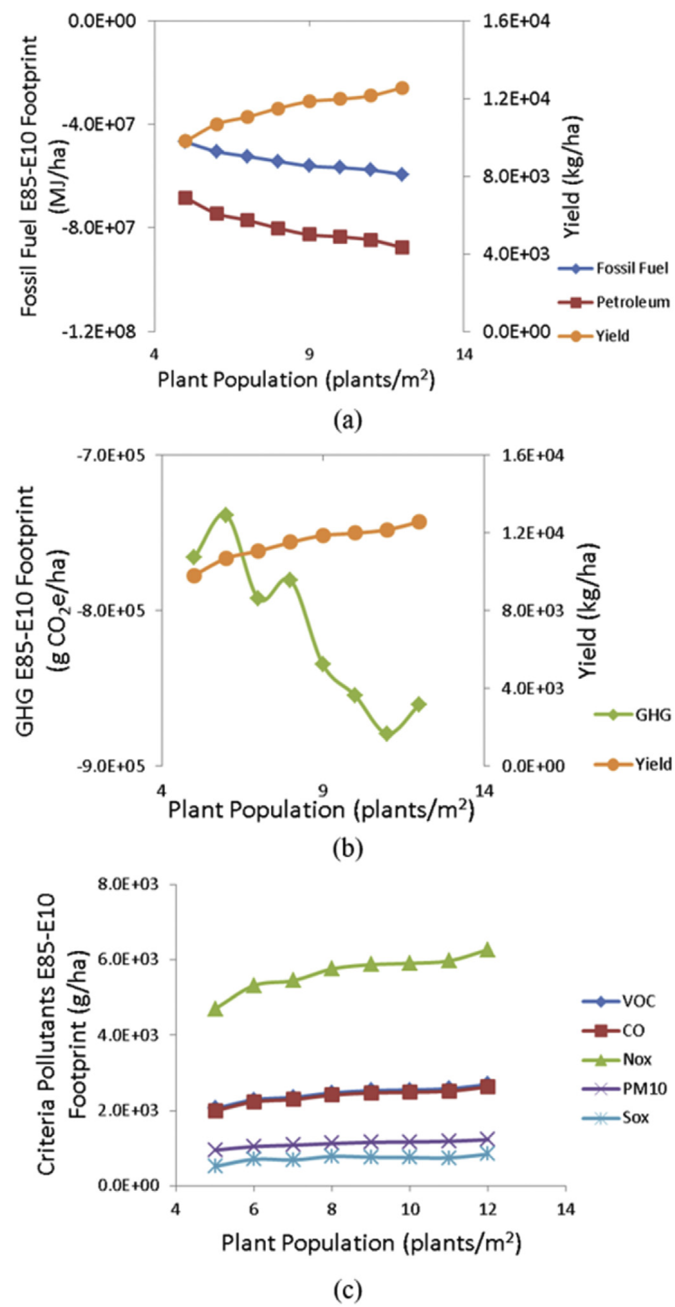

Fig. 8. E85-E10 footprint by plant population on (a) GHG emissions, (b) fossil fuels, and emissions and (c) criteria pollutants.

the decision maker may weigh the environmental trade-offs when determining plant population as it has differing effects on these categories.

While Fig. 8 uses predetermined nitrogen values for each plant population, Fig. 9 shows the relationships of GHG footprint to nitrogen fertilizer and plant population. The GHG footprint seems to be optimal with lower nitrogen application and higher plant population density. This seems to be the ideal decision for nitrogen application and plant density to provide the best GHG footprint within the system. The GHG footprint is highest when the plant population is very low and the nitrogen application is very high. This is because the low population density is not producing enough ethanol to offset GHG emissions created by the high fertilizer use.

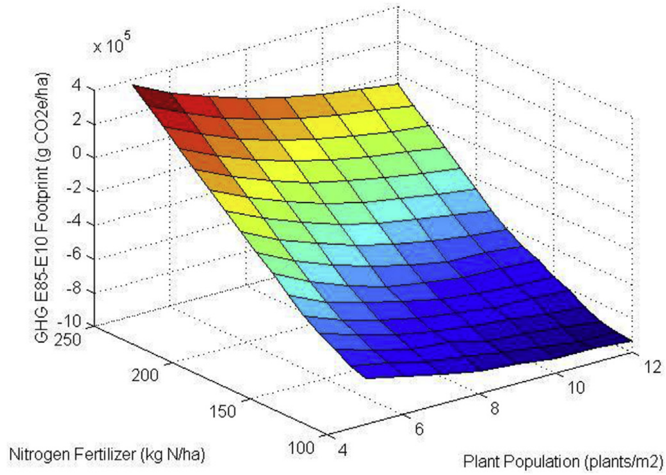

Fig. 9. GHG footprint vs nitrogen fertilizer application (kg/ha) and plant population (plants/m^2).

3.3. End user application

This program for integrating the crop and biofuel systems is primarily purposed as an environmental decision support tool. Both DSSAT and GREET have large user bases who use these tools to make informed decisions based on either production output or environmental impact (de Carvalho Lopes and Steidle Neto, 2011; Kopanos et al., 2017). Connecting the two creates a powerful tool that allows the user to do both and understand the impact that their decisions have on the integrated system. Many scenario analyses on the impacts of nitrogen fertilizer and plant population on corn growth have been done in the past. There are experimental field studies that test these variables against each other to determine their effect on grain yield for different years and different locations (Blumenthal et al., 2003). found a linear relationship between plant population density and grain yield and a quadratic relationship between total soil nitrogen and grain yield in Western Nebraska counties (Ping et al., 2008). studied the relationship between site-specific nitrogen and population density management and economic performance which showed little impact, though it did increase nitrogen use efficiency (Irmak and Djaman, 2016). concluded a positive relationship with plant population density and grain yield with mixed results for evapotranspiration. All of these results contribute heavily to understanding the effect that nitrogen application and plant population have on growth and economics of the farmer, but it is still in the closed system of the individual farming operation. This integrated tool provides a way to do these scenario analyses to understand not only how these variables can affect growth, but also the impact on emissions, resource use, and the environment when coupled with the ethanol system. This is a way to use the valuable crop research that is done to produce cropping models for the understanding of a larger system.

Likewise, LCA users will have a better understanding of the tradeoffs of using biofuels with a more functional corn farming pathway. GREET currently has a corn farming process included, but is limited in inputs. The default values are derived from USDA NASS data which averages management practices from regions of completely different climates and land. Integrating the DSSAT model allows the user to make GREET location-specific which can be a valuable tool for businesses that operate close to biofuel plants in various regions. Future work can include scenarios that run in different locations to analyze how different areas affect the environmental impact of producing biofuels. This study is focused on corn ethanol production in the Midwest but the corn-ethanol system is also prevalent in further stretches of the Great Plains and the South. A database could be created of these various locations and based on the weather and land differences.

The model can also run scenarios for various other biofuels. It includes biodiesel from soybean oil and ethanol production from corn stover, sorghum, and forest residue feedstocks. DSSAT includes models for soybean and corn stover production so additional scenarios can be run to better understand how these systems are interconnected in comparison to corn ethanol and reformulated gasoline. Corn stover is an important addition to the system as it is tightly connected to both the corn production and biofuel systems. Cellulosic ethanol plants are commonly found in the Midwest United States and can result in further emission savings from corn production. Residue from crop yields can be simulated using DSSAT and distributed to have a more accurate understanding of the emissions within this integrated system.

There are limitations to this tool, some of which are inherently attributed to the individual models. DSSAT's large user base mostly consists of researchers and scientists who do not make field decisions in hopes of selling their product. DSSAT is also limited as an irrigation scheduling tool. The automated irrigation setting does not give the user many options to adjust for strategies such as implementing deficit irrigation. GREET also does not incorporate irrigation pumping costs when calculating GHG emissions and energy use for the corn ethanol pathway. Many producers consider irrigation pumping a large expense, especially for drier regions where irrigation is required. GREET is limited to calculating direct emissions from each system and as a result, indirect emissions were not taken into account for this study. A user can add emissions from indirect sources, but this study focused specifically on the capabilities of the two models used. The framework allows for future work to explore the possibilities of adding indirect emissions from other models. GREET also does not consider methane emissions from irrigation and other agriculturally related emissions so those were left out of the scope of this paper.

This framework is also mainly a tool used for environmental assessment and does not include profitability. Decision makers are more likely to act based on their best financial interest even if there is an environmentally optimal solution. A more applicable tool will include economics in addition to environmental impact so that a user is more likely to use it.

Modelers and researchers have been developing and finding new ways to practically integrate agricultural production systems. This paper offers the methodology and framework for a tool that can connect two well-established models in their respective fields. In the generation where APIs and model wrappers are taking over the world of software and technology, it is important that agricultural models and software can keep up with this trend (Zhong et al., 2009). Programmers have made many tools to facilitate the connection of various programs which were utilized in this paper: the GREET API, the compiled DSSAT program, and the various Python packages used in the wrapper. The method also allows for the models to be automatically updated as the developers continue to work on the individual models. Other researchers may do similar studies and run their own holistic scenario analyses like how nitrogen fertilizer application was connected to total GHG emissions. This SOA offers users the ability to utilize these tools practically to make their own environmental assessments of corn ethanol scenarios. This framework makes the integrated model accessible for developers to create their own software, for decision makers to run their own scenarios, and for researchers to conduct analyses on this integrated system.

4. Conclusion

The DSSAT and GREET models were connected by running each program through APIs developed using Python. Several scenarios based on decisions that can benefit a user in studying what-if scenarios were run through this integrated model to identify the total environmental assessment of the full system. These scenario analyses can provide the user with a better understanding of the impact that certain key decisions, such as fertilizer application, can have on the environment and the rest of the system.

The DSSAT-GREET wrapper is not only a tool that can be used to evaluate and understand sustainability aspects of the system, but it also offers a step towards helping modelers and programmers make more effective decision support tools. Stakeholders in the crop and biofuel systems can better understand their effect on the other. Technology companies, large and small, develop APIs in the hopes of working together to make more powerful tools for society and a similar opportunity is available for environmental modelers. Future work will include integrating a model of a livestock system into the framework, incorporating other cropping systems, accounting for irrigation pumping costs, evaluating economic impacts, and developing an enhanced environmental impact assessment that includes other factors such as eutrophication and human health components. This integration will also be tested against long-term climate models and make system predictions for the future.

Acknowledgements

The authors thank the National Science Foundation (NSF) Innovations in the Food, Energy, and Water Systems (INFEWS) program for funding this work and other related projects under Award Number 1639478. The authors thank Deepak Kumar, University of Illinois at Urbana-Champaign for his work in verification of GREET model data.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.envsoft.2018.07.004.

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