Received: 30 May 2020 | Revised: 15 August 2020 | Accepted: 21 September 2020

DOI: 10.1002/aic.17113

PROCESS SYSTEMS ENGINEERING

AIChE JOURNAL

Meeting the challenge of water sustainability: The role of process systems engineering

Sirish L. Shah[1] | Bhavik R. Bakshi[2] | Jinfeng Liu[1] | Christos Georgakis[3] | Benoit Chachuat[4] | Richard D. Braatz[5] | Brent R. Young[6]

[1]Department of Chemical & Materials Engineering, University of Alberta, Edmonton, Alberta, Canada

[2]Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, Ohio

[3]Department of Chemical & Biological Engineering, Tufts University, Medford, Massachusetts

[4]Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, UK

[5]Department of Chemical Engineering, MIT, Cambridge, Massachusetts

[6]Department of Chemical and Materials Engineering, University of Auckland, Auckland, New Zealand

Correspondence
Christos Georgakis, Department of Chemical & Biological Engineering, Tufts University, Medford, MA 02155.
Email: christos.georgakis@tufts.edu

Abstract

This white paper is the result of discussions during the FIPSE-4 conference (http://fi-in-pse.org) in June 2018. It aims to highlight open problems and provide directions for future research in the area of water with emphasis on its agricultural usages. Some of the open problems discussed are: (a) the use of ecosystems as unit operations to understand their role in providing freshwater and in cleaning polluted water; (b) consideration of interactions and independencies between flows of water and other resources, such as food, energy, materials, ecosystem services, and environmental emissions; (c) challenges in modeling, sensing, and closed-loop control in precision irrigation. In particular, the development of agro-hydrological models that balance computing speed versus solution details and accuracy: (d) The use of state and parameter estimation approaches, through field measurements, to obtain soil moisture levels accurately; and (e) decision support systems to administer water and nutrient needs for optimum yields of agricultural products.

KEYWORDS

control, estimation, mathematical modeling, water

1 | INTRODUCTION

Water is essential for our daily life. As Michel Jarraud, former Chair of the United Nations Water, stated in the 2015 World Water Development Report[1]: "*Water is truly at the core of sustainable development. It is inextricably linked to climate change, agriculture, food security, health, equality, gender, and education, and there is already international agreement that Water and sanitation are essential to the achievement of many sustainable development goals*." While about 70% of the Earth's surface is covered by water, less than 2.5% of it is fresh water. The agricultural, industrial, and domestic water needs of the fast-growing world population are already exceeding the currently available freshwater supply. The challenge of ensuring water and food security has been consistently recognized as one of the most significant global risks by the World Economic Forum over the past decade.[2,3] According to a recent statistical analysis of water consumption data conducted by the United Nation's Food and Agriculture Organization (FAO) (Figure 1), agriculture and industry are the two most significant water users, accounting for almost 90% of all freshwater consumption. Population growth is the primary factor causing the global water supply crisis.[2] In addition to population growth, climate change and pollution are also important causes of the water supply crisis. The challenges of insufficient water quantity and poor water quality are prevalent widely across most nations of the world. These challenges are depicted in Figure 2 for water quantity and in Figure 3 for water quality. Figure 2 shows the projected water scarcity in 2030 under a business-as-usual scenario, indicating that there will be hardly any populated areas of the world that will not face water scarcity, which is defined as the ratio of the Water withdrawn for human use to the Water available in the watershed. In many developed economies, the industry is a large user of freshwater, including activities such as thermoelectric power generation and heating, cooling, and dilution needs in other sectors. Methods for reducing the use of process water are available and have been widely adopted in process design.[6] However, many such methods aim to optimize a monetary objective such as profit or net present value (NPV). Since Water is often underpriced or even free, such designs may not be capable of dealing with increasing water scarcity that is conveyed in Figure 2.

The most substantial use of freshwater is in agriculture. As shown in Figure 1, agriculture consumes about 70% of the global freshwater withdrawals.[1,4] As population growth continues, 60% more food will be needed to satisfy the demand of more than 9 billion people worldwide by 2050. In many regions rich in Water, such as the United States and Canada, Water allocated to irrigation is mostly capped or will be capped soon.

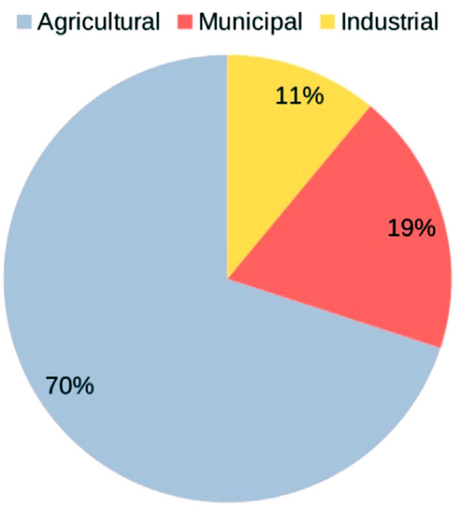

FIGURE 1 Worldwide water consumption statistics in 2016 based on data from FAO[4] [Color figure can be viewed at wileyonlinelibrary.com]

Any further increase in irrigated acres needs to come primarily from improvements in water efficiency.[7-9] Policies related to water conservation and new technologies clearly need to be developed for more efficient water consumption; otherwise, "water scarcity" will become a global issue soon. Agriculture consumes the most significant portion of freshwater withdrawals. At the same time, the average water-use efficiency worldwide is still low, estimated to be about 50–60% 10 years ago.[10,11] Consequently, agriculture offers the best opportunity to minimize waste and improve the efficiency of food production for a growing world population that has already surpassed 7 billion.

In many parts of the world, water quality also presents many challenges. Many conventional water pollutants such as in untreated sewage and industrial Water have been addressed with the help of environmental regulations and policies, at least in developed countries. These have encouraged modifications in manufacturing processes and the use of many waste treatment technologies. However, other water pollution challenges remain. For example, Figure 3 shows the locations of hypoxic zones (where the oxygen concentration is so low that animals can suffocate and die) across the world's oceans, which are created due to excessive nutrients in the sea. This excess is caused by fertilizer runoff from farms and lawns, and due to untreated sewage. This problem also appears in freshwater bodies such as lakes and rivers, and groundwater. In many parts of the world, emerging pollutants such as endocrine disruptors (chemicals that cause hormonal imbalance in the body) and microplastics pose new challenges. Pollution due to plastics in water bodies is attracting societal attention. It is resulting in a backlash in the form of bans on single-use plastics and efforts to avoid plastic products. Many industries are working toward a net-zero or net-positive water use. To achieve this goal, direct and indirect water use (virtual water, water footprint), and water sustainability in watersheds,

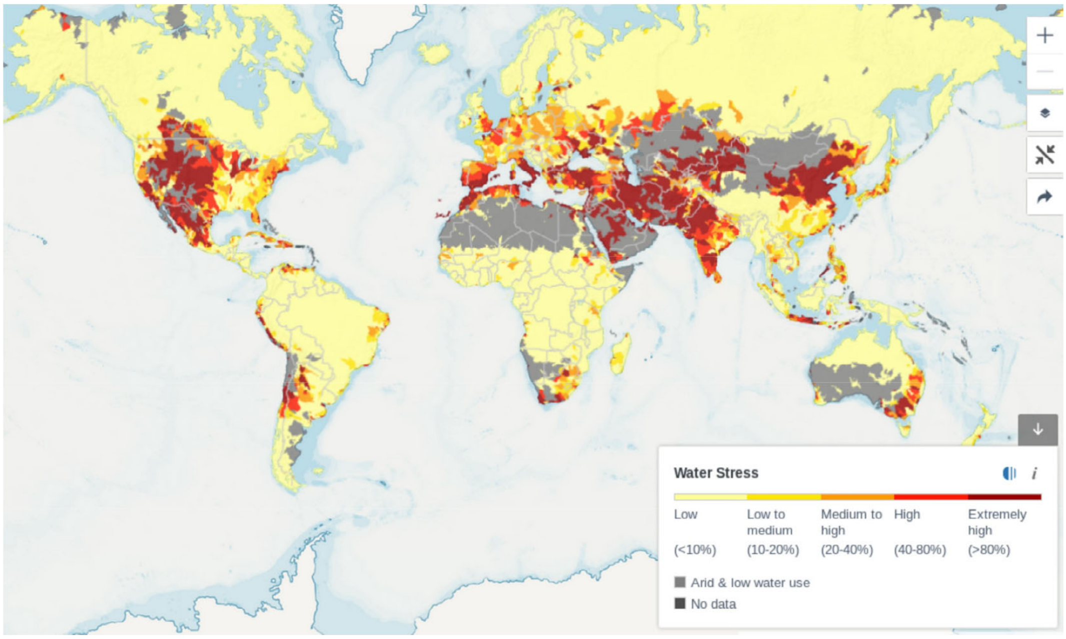

FIGURE 2 Projected water stress in 2030 under business as usual scenario. With permission from WRI aqueduct (http://wri.org/aqueduct) [Color figure can be viewed at wileyonlinelibrary.com]

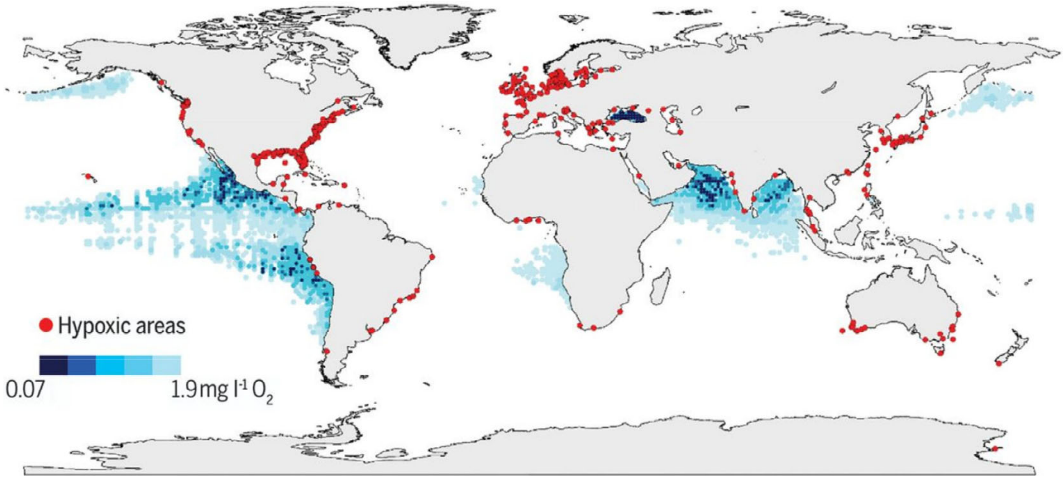

FIGURE 3 Areas of low ocean oxygen concentration and hypoxia Breitburg et al.[5] Used with permission [Color figure can be viewed at wileyonlinelibrary.com]

need to be considered. Changes in land use and climate are likely to worsen the quantity and quality of water.

This paper provides a perspective on the role that process systems engineering (PSE) should play in meeting the challenges of water sustainability. The focus is on the possible future innovation and the resolution of many of the open research problems in the broad areas of Water and agriculture. The next section describes some of the environmental issues and motivates the need for the use of systems engineering approaches. It is followed by a description of specific areas where the PSE community could contribute. The section includes the use of process control to improve the efficiency of agricultural water use, approaches for process and supply chain design, and the importance of considering the nexus between food, energy, water, and other factors. The last section summarizes the key insights and conclusions.

2 | ROLE OF PSE

Without a systems view, it would not be possible to meet the goals of water sustainability. This perspective is needed because environmental problems tend to shift across space, time, types of flows, and disciplines.[12] For example, electric cars do not have emissions but shift them upstream to the power generation process. Encouraging some biofuels may reduce carbon dioxide emissions in the short-run but may cause deforestation, which causes increases in atmospheric CO_2 in the long run. Improving water quality and reducing its consumption may require greater energy use for purification and reuse; improvement in the efficiency of consumer goods such as cars and light bulbs may decrease their cost and encourage consumption and environmental impact. Thus, to truly solve ecological problems, such shifting should be avoided or studied, which is possible only with a systems view. Recent efforts have expanded the boundary of PSE by incorporating the approach of life cycle assessment (LCA).[13-15] This approach can account for shifts in space and between types of flows. However, reducing the chance of changes in time and across disciplines requires further expansion to include effects of the markets and economy, and human behavior while accounting for spatial and temporal variation.[16] Focusing only on water sustainability may also be too narrow, and other environmental impacts should also be considered.

In addition to reducing the chance of shifting environmental impacts, sustainability also requires respect for nature's capacity to supply goods and services on which human activities depend. Most disciplines do not take nature's capacity into account. Still, recent interest in ecosystem goods and services is resulting in frameworks such as techno-ecological synergy (TES)[17] to address this challenge. Thus, for PSE to contribute to meeting the challenges of water sustainability, it needs to expand its reach to include the role of ecosystems in providing Water and regulating its quality.[16,18]

These requirements present many opportunities and challenges for future innovation in PSE. They present new types of challenges in design and control problems related to using Water efficiently in large-scale systems, such as industrial sites, farms, and cities. Accounting for ecological carrying capacity requires approaches to work with nature's intermittency by respect for its limits while meeting technological goals in a resource-efficient manner. Designs that reduce life cycle water use or water footprint,[19] along with maximizing profitability in a socially acceptable way, require advanced optimization methods and integration with models of ecological and economic systems. Seeking synergies with ecosystems can also result in innovative solutions that will pose unique challenges for their design and operation. Some such opportunities for future innovation are described in the rest of this paper.

3 | RESEARCH PROBLEMS AND OPPORTUNITIES FOR FUTURE INNOVATION

3.1 | Process control in precision irrigation

Traditionally, the focus of agricultural water management is more on meeting regional demands; however, the water “ecosystem” needs to

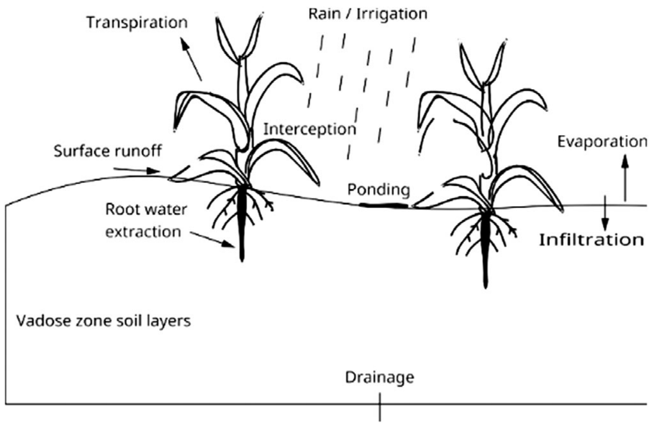

FIGURE 4 An agro-hydrological system

be examined in a broader context. In general, less attention has been given to on-farm water applications. With the increasing pressure on improving overall water efficiency, it is becoming more and more important to consider the on-farm water-use efficiency by representing plants and crops as agro-hydrological systems. An agro-hydrological model characterizes the hydrological cycle between soil, atmosphere, and crop. For irrigation applications, it is typically only necessary to consider the vadose zone (which extends from the top of the ground to the water table) of the soil that is above the water table. As a result, underground water flow is not considered. Figure 4 provides a simple illustration of an agro-hydrological system. In the agro-hydrological system, water transportation takes place primarily utilizing rain, irrigation, evaporation, transpiration, infiltration, root water extraction, surface runoff, and drainage. At the surface, when there is rain or irrigation, Water may enter the soil depending on the soil moisture condition. When the soil is unsaturated, Water infiltrates into the ground; however, when the soil is saturated, the infiltration tends to cease, and ponding starts to occur. After a certain ponding height, the water level breaks, and runoff starts to happen. Some of the rain or irrigated Water may not even reach the soil surface. Within the soil, the roots of the crop act as water sinks that extract Water from the soil.

The advances of various technologies, including agro-hydrological system modeling, numerical solution of agro-hydrological models, and remote sensing in the past years, have made it possible to consider on-farm water-use efficiency from a systems' perspective. These advances have been achieved primarily due to the collaborative effort between various research areas including, for example, hydrology, meteorology, environmental engineering, soil science, geo-statistics, transport phenomena, and agricultural water management. PSE can provide a holistic systems perspective on these issues and help integrate these different disciplines to provide a framework for modeling and closed-loop control, which can maximize irrigation water-use efficiency and—at the same time—take into account other considerations (such as costs) and constraints (environmental regulations, crop properties). In recent years, attempts to integrate these technologies to form closed-loop irrigation systems to improve irrigation water-use efficiency as well as to reduce energy consumption and to improve crop yield for greenhouses and vineyards have been made.[20] These solutions are in what may be termed as "controlled" environments. There is a need for a broader framework of solutions that consider the dynamics of crop-specific agro-hydrological systems in heterogeneous soil conditions and combine them with the environmental requirements and constraints, especially for larger agricultural fields.

Irrigation science dates back to early history when people started to grow crops. While modern irrigation technologies have been adopted in many developed countries, traditional irrigation methods are still widely used in many parts of the world. The current irrigation methods can be classified into two categories: traditional and modern techniques. The traditional irrigation methods mainly involve surface irrigation, where irrigation water is flooded over the crop field, or Water is passed through furrows. On the other hand, drip irrigation and sprinkler-based irrigation are the two most popular modern irrigation methods. For drip irrigation, Water is irrigated close to crop roots. Drip irrigation is somewhat costly and only used in small vegetable fields, orchards, or vineyards. For sprinkler-based irrigation, irrigation water is sprayed over the crop through sprinklers. A sprinkler may be installed as a stand-alone unit or be mounted on a rotating pivot, called the central pivot. For larger fields, central pivots are more common. Figure 5 shows a classification of the different irrigation methods.[21]

In the current agricultural irrigation practice, the amount of water to be irrigated and the time to apply the irrigation are determined in advance based on the irrigators' (typically the farmer's) knowledge. The actual conditions in the field are generally not considered in determining the irrigation amount and time. Thus, from a PSE perspective, the current irrigation practice is an *open-loop* decision-making process. The information flow of open-loop irrigation is shown in Figure 6. However, it is well recognized in process control that open-loop control is quite imprecise. Namely, open-loop irrigation generally leads to either over-irrigation or under-irrigation.

Precision irrigation technologies have been advocated as the means to meet the challenges of water sustainability. Consequently, there has been ever-growing research interest in precision irrigation. From the PSE perspective, the key is to close the decision-support loop and form a *closed-loop* system for precision irrigation. In the closed-loop system, sensing instruments (e.g., soil moisture and nutrient sensors, evapotranspiration (ET) gauge, thermal cameras on drones, or satellite imagery data) can be used to collect various real-time field information regularly. The different pieces of information can then be fused to estimate the entire field's conditions. The estimated field conditions could then be fed back to a self-learning control system. The self-learning control system would then calculate the best irrigation commands for the next few hours or day(s) based on a field model, the estimated field conditions, local weather forecast, as well as other pre-specified irrigation requirements. Figure 7 shows a schematic of the building blocks of a possible closed-loop irrigation system. Due to significant nonlinearities, uncertainties, and the large scale of agricultural fields, there are significant challenges in modeling,

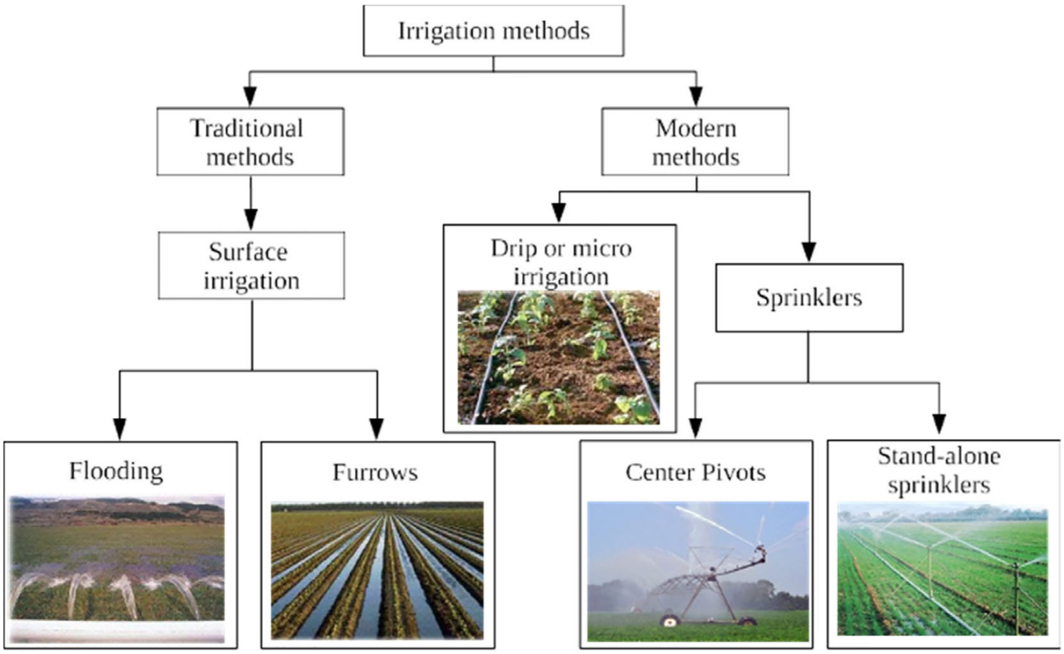

FIGURE 5 Classification of irrigation methods [Color figure can be viewed at wileyonlinelibrary.com]

FIGURE 6 Open-loop irrigation

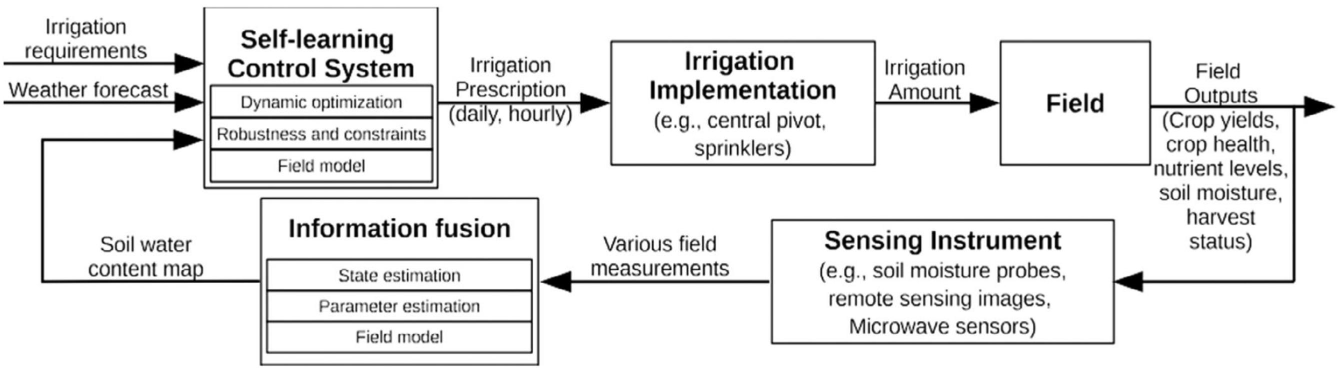

FIGURE 7 Block diagram of a possible closed-loop irrigation system

sensing, estimation, and control algorithm development that need to be addressed.

3.2 | Agro-hydrological models

The dynamics of soil water content inside the soil can be described by the Richards equation[22]:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K \nabla H) - S \tag{1}$$

where θ (cm^3/cm^3) is the volumetric soil water content, t (hr) is the time, K (cm/hr) is the unsaturated soil hydraulic conductivity tensor, H (cm) is the hydraulic head, and S (hr-1) is a sink term that accounts for root water extraction. The Richards equation describes Water flow inside the soil and includes irrigation through the top boundary condition, which makes the Richards equation having a varying temporal and spatial top boundary condition. A crop model can be integrated with the Richards equation through the sink term to reflect the crop's water requirements.

One common approach for modeling crop water requirements is based on the ET rate of the crop with respect to a “reference” crop, as described in Allen et al.[23] The ET rate is a combined term of evaporation and transpiration. Evaporation accounts for the water loss of the surrounding exposed soil. In contrast, transpiration is the process of water movement inside the crop and its evaporation from the aerial parts, such as leaves, stems, and flowers. Ideally, the amount of Water transpired is equal to the root water extraction so that a water balance is achieved in the crop. The Penman–Monteith equation is commonly used tool for approximating ET values based on hourly weather data.[23] The numerical solution of the Richards equation is, in general, quite challenging due to the nonlinearity of soil properties (e.g., dramatically varying hydraulic conductivity *K* when soil moisture changes), varying top boundary conditions, and the large scale of the typical problem. The foundation of a precision irrigation system would require models of the agro-hydrological system that calls for solutions to several open problems that are discussed below.

- There is a strong need to balance the computing speed, numerical robustness, and solution accuracy when solving the Richards equation. One of the most crucial factors affecting the solution accuracy is the grid size. Under some extreme conditions such as arid soil, partially saturated soil, and highly heterogeneous fields, the problem becomes stiff, and the grid size should be relatively small to capture the dynamics, which significantly increases the computational load. The high degree of nonlinearity and uncertainty in model parameters of the Richards equation also substantially affect its solution. Adaptive spatial discretization and adaptive temporal discretization could be used to decrease the size of the computational nodes while maintaining solution accuracy. Another approach to establish a balance between computing speed and solution accuracy is to parallelize the computational task. One way is to develop distributed subsystem models and account for the interaction between them. The high degree of nonlinearity at unfavorable conditions may be overcome by approximating the unfavorable dynamics with a data-driven identified model. The accuracy of the model parameters can be improved by using state and parameter estimation techniques, which will be discussed in the following section.
- The design of a closed-loop irrigation control system requires not only the soil water dynamics model but also a model of the irrigation implementation system (central pivots and sprinklers), crop type and local weather systems. A model of the irrigation implementation system should take into account the rotation speed, the fluid dynamics, and the maximum irrigation rate of the central pivot. A weather model can be used to predict future weather conditions based on historical measurements or meteorological predictions. A dynamical model of the crop should consider the crop structure, root structure, biomass of the crop, and crop yield as a function of time, soil moisture content, weather conditions, and so forth. These models are useful in simulating the entire control system and assessing the performance of a control system before implementing it. These models are also helpful if a predictive control algorithm, such as model predictive control (MPC),[24] is used. The integration of these models into one system should also be investigated.
- The Richards equation is widely used in modeling soil water dynamics. However, when soil heterogeneity is present, significant challenges exist in numerically solving the corresponding equation. Other modeling approaches should also be investigated. Besides the Richards equation, there are some other simpler models, such as the AquaCrop model and the Soil and Water Assessment Tool (SWAT) model.[25,26] These models are based on simple water balance methods. The advantage of using these models is that they are computationally less complex and linear. The disadvantage of using such models is that they do not accurately represent the complex dynamics of Water in the soil. Another alternative modeling approach, other than the Richards equation, is to use data-driven models consisting of neural networks or identified based on machine learning methods. One limitation of using data-driven models in the agro-hydrological system is the availability of sufficient quality training data about the root zone soil moisture, covering all the possible scenario. One possible intermediate solution is to use a data-driven model for the surface moisture content and the Richards equation to describe the flow in the vadose zone.

3.3 | Sensing agro-hydrological systems

The ability to measure soil moisture is critical in the development of any closed-loop control system for agro-hydrological systems. In soil labs, the most common method to determine soil moisture is the gravimetric method with oven drying. While the gravimetric method is one of the most reliable, it is not appropriate for real-time monitoring of soil moisture. For agricultural field applications, a variety of techniques have been developed to measure soil moisture indirectly, with the most mature and reliable being sensors for point measurements. These sensors need to be buried in the soil and provide soil moisture measurements at specific point locations. Most of these sensors provide the soil water content information based on measuring the dielectric permittivity of the soil.[27] These sensors have the advantages of portability, easy installation, and operation, the ability to measure soil moisture at different depths. However, they can only provide measurements for a limited number of point locations, are expensive and, to some extent, destructive due to, for example, wiring to deploy.[28]

Non-invasive sensing techniques provide a more feasible approach to capture the spatial variability of soil moisture. One such non-invasive technique relies on signals propagating from a transmitter through the soil to a receiver or reflected from the soil to the receiver. Other useful signals are the ones emitted naturally from the soil to the receiver. Ground-penetrating radar, passive microwave sensors, or radiometers are two examples of such non-invasive sensing techniques. The surface soil moisture may also be obtained using optical and thermal remote sensing techniques. Optical remote sensing deals with the relationship between soil moisture and soil spectral reflectance. The thermal remote sensing methods, in general, estimate soil moisture based on either the thermal inertia method or the temperature index method.[28] These non-invasive instruments may be mounted, for example, on a central pivot to provide a regular scan of a field.

Research challenges relevant to agro-hydrological system sensing are:

- Soil moisture remote sensing techniques have the advantage over point sensors in that they can capture the spatial variability for a large field. There are some challenges to estimate the surface soil moisture using remote sensing methods. First, there is no practical method to handle the surface roughness and vegetation in the estimation of surface soil moisture from remote sensing images. Second, the accuracy and resolution of remote sensing are not very high. A combination of different types of sensors, including high-resolution microwave sensors, thermal and optical remote sensing, and point sensors, may provide a feasible approach to overcome the shortcomings of each sensing method.
- Image-based sensors from drone surveillance and satellite image data can be used to assess various measures of a field such as crop health, crop maturity, time to harvest, canopy moisture levels. Such sensors would require calibration. The preliminary first step would be to archive images and combine this information with regular field measurements of moisture, crop health, soil nutrients and then build appropriate soft sensors relating the remote measurements to actual conditions in the soil. The collection of image data and field measurements is a necessary first step to develop such advanced soft sensing technology. The field measurements would have to be obtained at specific or random locations in such a spatiotemporal system. The location of where to take such measurements is in itself an open problem.

3.4 | Parameter and state estimation for agro-hydrological systems

One major barrier in developing a closed-loop irrigation control system is the availability of proper soil moisture data. Generally, it is not feasible to have s single sensing instrument covering an entire agro-hydrological system given the typical size of an agricultural field. An alternative is to estimate the soil moisture using state estimation techniques. The most commonly used state estimation algorithms include the Kalman filter and its variants.[29] Due to the complexity of agro-hydrological systems, the model-data mismatch is a widespread occurrence in soil moisture estimation. Incorrect soil hydraulic parameters may lead to persistent bias in soil moisture estimates. This indicates the importance of accurate soil parameters in soil moisture estimation. Soil hydraulic properties may change slowly over time, and parameter estimation (often referred to as inverse modeling in the soil modeling community) provides a way to capture this. Parameter estimation is also very often considered simultaneously with state estimation for agro-hydrological systems.[29,30] For a large-scale agricultural field with heterogeneous soil properties, it may lead to an estimation problem with too many parameters to estimate, render the problem unobservable, and pose significant numerical and computing challenges.

Some of the open parameter and state estimation challenges that need to be addressed are:

- In the existing literature, the Kalman filter and its variants are the most commonly used filtering/estimation methods. In these methods, constraints on the states are, in general, not considered. Constraints on soil moisture are indeed very crucial in state estimation because if the estimated soil moisture enters extreme conditions such as saturation zone or arid zone, the efficiency and accuracy of the model can deteriorate, and the estimator may even become unstable. Estimation methods that can take constraints into account explicitly, such as moving horizon estimation (MHE), may be considered to address this issue. However, if MHE is used, its high computational complexity may be a formidable challenge.
- In irrigation control, the availability of root zone soil moisture is of most importance. Moisture measurements on the soil surface ever a wide field, obtained from remote sensing, can provide useful information in estimating root zone soil moisture. However, the accuracy of image-based remote sensing is typically not as accurate as point sensors. On the other hand, point sensors generally are more accurate, but it is infeasible to deploy many of them to cover an entire field. As discussed earlier, a combination of different types of sensors should be considered, which implies that estimation algorithms that can take various measurements with various accuracies into account need to be developed for agro-hydrological systems.
- State estimation is essential in reconstructing the state (soil moisture) information across the entire field, which is vital for irrigation decision making. While there are many existing results on parameter and state estimation of agro-hydrological systems, two major relevant questions have not been addressed. What is the minimum number of sensors required for estimating the soil moisture of the entire spatial–temporal system, and where are the best locations to place the sensors? Given the size of typical agricultural fields, these are not trivial questions. In Nahar et al.[30] and Sahoo et al.,[31] observability analysis and degree of observability were demonstrated to be useful tools for determining the minimum number of sensors as well as their optimal location. However, Nahar et al.[30] and Sahoo et al.[31] only considered point sensors. Further research should be conducted to take various types of sensing instruments for soil moisture into account. The cost and precision of the sensing instrument should also be considered.
- While initial soil parameters may be determined in a soil lab with soil samples, soil properties change slowly over time due to topology changes, crop growth, and so forth. Taking soil samples frequently is expensive and time consuming, especially when the

investigated field is large and has various soil types over the field. Simultaneous parameter estimation, together with soil moisture, provides a cheaper and feasible way to capture the time-varying nature of soil properties. The estimation of multiple soil parameter estimation is one of the essential factors for the success of model-based closed-loop irrigation.

- Furthermore, soil heterogeneity is one of the biggest challenges, as it requires more parameters to be estimated, which leads to increased computational complexity and numerical difficulties. In addition to soil heterogeneity, parameter identifiability should be investigated. It is one of the unexplored topics in soil parameter estimation and is also related to sensor placement. A parameter identifiability analysis can indicate how many measurement points are needed for accurate parameter estimation and the maximum number of parameters that can be identified.

3.5 | Irrigation water management

In the literature, there are several results on closed-loop irrigation. For drip irrigation, most of the existing results rely on simple on–off control and point sensor measurements. It has been demonstrated that a closed-loop drip irrigation system can lead to significant water conservation compared with traditional irrigation methods.[32,33] Closed-loop drip irrigation was also reported to lead to improved quality and quantity of flowers, shorter growing season, and decreased electricity usage.[34] For larger-scale agricultural fields, sprinklers mounted on central pivots are typically used for irrigation. Figure 8 shows one example of a central pivot. The controller design for this type of irrigation system is much more complicated. Whereas in existing studies, the spatial variation of soil moisture is often not explicitly considered. Several challenges related to the control system design are discussed below:

- An agro-hydrological system is a large-scale system. After discretization, a model may have thousands of discretized states. It is typically infeasible or not practical to handle such systems directly in the design of state estimation and real-time control systems. Model reduction should be performed. Model order reduction is a widely accepted technique to handle complex processes such as chemical plants. There are different existing model reduction methods, including, for example, proper orthogonal decomposition, optimal Hankel norm reduction, balanced truncation methods.[35] However, these methods cannot preserve the topology of the original system. That is, the states of a reduced model may not be physically meaningful. To capture the spatial heterogeneity of an agro-hydrological system, one should have reduced-order models that preserve the spatial distribution of soil types across the entire field. This is an important task that requires spatial variability information such as determination of the optimal sensor placement,[31] subsystem decomposition for distributed estimation and control designs.
- When dealing with irrigation control of large-scale agricultural fields, as mentioned earlier, central pivots equipped with sprinklers are widely used. A central pivot is a circular irrigation implementation system consisting of several segments of sprinkler-equipped pipe supported by wheeled towers. The pipe slowly rotates around a fixed pivot to perform irrigation. A central pivot takes about one to 3 days to go through an entire circular field once, depending on the size of the field. A central pivot is a slowly moving actuator of an irrigation control system. For a specific circular segment of a field, it has access to irrigation/control only for a limited amount of time everyone to 3 days. A predictive model of the system would be very useful in optimizing the irrigation commands while taking this control availability constraint and weather forecast information into account. MPC[24] could be a favorable control algorithm given its ability to use model and handle state and input constraints.
- When MPC is used in closed-loop irrigation control, its high computational complexity for large-scale nonlinear systems should be carefully considered. Model reduction, as discussed above, can be useful in reducing the computational complexity of nonlinear MPC.

FIGURE 8 A 1-segment central pivot. The length of the arm is 50 m. A typical central pivot usually has a few segments with the total arm length about 300 to 400 m [Color figure can be viewed at wileyonlinelibrary.com]

However, for nonlinear systems, model reduction often is not sufficient in reducing the computational complexity of nonlinear MPC.[36] Model linearization, such as trajectory piecewise linearization, may be used jointly with a model reduction to obtain a computational efficient MPC algorithm.[36] Linear time-varying models identified from input–output data can also provide a feasible solution.[37] In addition to model reduction and linearization, distributed MPC offers another possible solution.[38]

- Some other vital issues should be considered in the design of irrigation control systems. One such challenge is the design of robust control algorithms. There will likely be a significant model-plant-mismatch given the challenges in agro-hydrological system modeling and the time-varying nature of agro-hydrological systems. Other than model-plant- mismatch, the uncertainty in weather conditions such as wind speed and temperature should also be considered. Typically, only the regional weather conditions are available through a regional weather station. There can be non-negligible mismatches between the weather conditions of the micro-climate of a specific agricultural field and its corresponding regional weather forecasts. Some other issues that should be considered include the cost of implementing such a closed-loop irrigation control system and the ease of use of the control system.

3.6 | Batch process monitoring and control of agronomic processes

A contemplative paradigm shift could be considered by treating each crop growth sequence as a batch PSE process. By using agro-hydrological models that are crop- and zone-specific, consider, as an example, the average 3 to 4-month growth cycle of wheat or corn plants from sowing to harvesting, which is a batch process with time-varying dynamics. During this batch growth cycle, decision support systems have to be developed to administer water and nutrient needs for optimum process yield, just as in classical "chemical" batch processes, as illustrated in Figure 9.

For such a 'batch' type process, Water, nutrient, and monitoring needs for optimum crop yields at harvest time would require:

- An initial image analysis during tillage to determine water and nutrient levels before seeding.
- After that, regular measurements of soil moisture in the vadose zone carried out with a fusion of additional information from weather data and local micro-climate sensors.
- Seedlings in their early growth stage, would be quite vulnerable and require monitoring and detection of pests and diseases.
- Normal growth and health monitoring of the main crop and to also detect weeds and identification of weed types; if weeds are detected in specific areas, then only those areas need to be treated for weed control rather than the entire field.
- Assessment of plant nutrients from leaf canopy to monitor water and fertilization needs, which may have to be crop-specific and also zone-specific even in a single field due to heterogeneous soil conditions and the applicable micro-climate in the local areas. The spatial resolution of aerial images has to be fine (centimeters per pixel) to detect leaf color changes of crops and also identify plant stress causes due to water stress or poor soil nutrients. The images should be able to detect if this is widespread or prevalent only in specific areas for water and fertilizer applications to the relevant areas. Development of decision support systems based on information fusion from all physical and soft sensors for prescriptive Water and nutrient needs of the crops for optimum yields.
- Prediction and planning of harvest times to help in subsequent supply-chain planning for processing and transport to markets.
- Moisture and nutrient monitoring would also be carried out at various stages of post-harvest to determine residue nutrients that would then be the initial starting point for a new batch of crops.

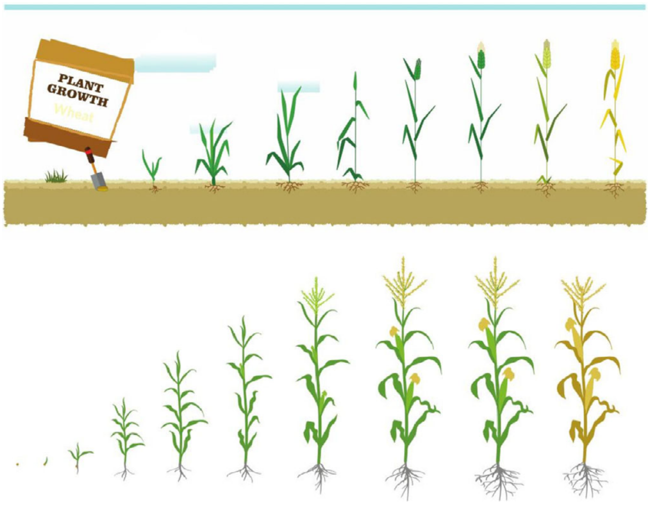

FIGURE 9 Images to illustrate "batch" type growth sequence from sowing to harvesting of two widely grown crops: wheat (top image) and corn (bottom image). At various stages of growth, the soil moisture in the root and vadose zone plus crop health would have to be monitored for water and nutrients needs to optimize yield [Color figure can be viewed at wileyonlinelibrary.com]

All of these monitoring methods would require the development of new sensors. Aerial sensing using drones with broadband spectra (light and infrared waves), as illustrated in Figure 10, is one possible solution that would have to be carefully explored. Such techniques may require unfolding each image and analyzing the RGB + IR pixels and have these calibrated with manual terrestrial measurements taken at selected points. Such data would eventually allow the development of a moisture, nutrient, and "plant health" soft sensor based on drone images with timely bias updates from terrestrial sensors. Such sensing methods are likely to be crop-specific and will also vary with time and space from seedlings to crop maturity. The development of these sensors will require a collection of many months of image data plus soil moisture and nutrient samples taken throughout the growth cycle of the crop.

FIGURE 10 Agriculture drones with centimeters per pixel resolution cameras can be trained to detect changes in leaf color to infer water and nutrient needs of crops. Computer vision methods can be developed to detect and identify different weed types [Color figure can be viewed at wileyonlinelibrary.com]

This is a challenging "BIG" agronomic data sensor fusion project that would require the extraction of many pieces of information. These might include aerial (drone) imagery, weather data, and soil analysis from local field measurements. All of the data need to be collected over many months from sowing to harvesting. At the same time, residue soil analysis might also be needed. Machine learning algorithms must be used in analyzing such vast volumes of geospatial agronomic data. The entire agro-hydrological system has to be considered as a non-uniformly sampled spatiotemporal system for which feedback algorithms have to be designed for precision and optimal crop production. The ultimate goal should be to grow better crops with less Water, less fuel, less fertilizer, and fewer pesticides and herbicides. The multiscale nature of the entire cycle from sowing to harvesting plus supply chain issues for processing the crop yields for markets will also needs to be considered in a systems framework.

3.7 | Water-saving strategies for public parks

Aside from agriculture, a significant amount of Water is used for maintaining lawns, parks, and sports fields. In Milesi et al.,[39] it is reported that the Water used for these outdoor green spaces ranges between 22 and 38% of the total residential water consumption in cool climate regions and between 59 and 67% in hot climate regions across North American cities. The total lawn area in the United States is about 1.5% of the overall country size, translating to 1.2×10^6 km^2, which is significant. Therefore, improving the irrigation efficiency for lawns, parks, and sports fields is also important. In some locations, replacing lawns and other non-indigenous land cover by ecologically appropriate vegetation can also be a sustainable way of reducing water use while enhancing ecosystem services and biodiversity.

Increased urbanization and reduced natural vegetation have led to significantly increased stormwater volumes. Stormwater is typically collected using the city drainage system and is either stored in stormwater ponds or discharged to downstream water bodies. The reuse of stormwater in irrigating city green spaces such as parks, sports fields, and green roofs is advocated for sustainability. When stormwater is used for irrigating neighboring parks or sports fields, it can be used to reduce the amount of tap water used for irrigation. In this case, stormwater storage ponds are managed near to its source, which reduces the chance of flooding in downstream areas. The interplay between the stormwater storage ponds, tap water consumption, and green space water needs poses many challenges in modeling and control system design. One such example is Nahar et al.,[40] in which a closed-loop scheduling problem is studied to understand the interplay between stormwater pond level and irrigation scheduling. Some related challenges are:

- For residential lawns, parks, and sports fields, there is a strong need to develop easy-to-use and affordable sensing and irrigation implementation devices. For the grasses used for residential lawns, parks, and sports fields, the root zone is typically shallow. Soil surface moisture measurements should be sufficient to reflect the Water contained in the root zone. Remote sensing based on cameras mounted at fixed locations or drones could be very useful in obtaining soil surface measurements. It is also necessary to develop smarter sprinklers such that the water flow rate and direction can be adjusted in real-time. The majority of the existing sprinklers for lawns are powered by water pressure, and the Water flow rate and direction cannot be adjusted in real-time, which greatly restricts the degree of controllability of the entire irrigation system. When developing the sensing and implementation devices (especially for residential lawns), ease of use and affordability should be two important considerations.
- Using stormwater for irrigating parks or sports fields adds more degrees of freedom into the stormwater management system, particularly in the management of the level of the neighborhood stormwater storage pond under extreme weather conditions. The

level of a stormwater storage pond should be maintained within the allowed minimum and maximum values. As illustrated in Nahar et al.,[40] when stormwater management and irrigation are considered simultaneously, the stormwater management performance may be significantly improved in terms of avoiding pond overflow or drying out. A predictive model characterizing how irrigation and precipitation affect the level of the storage pond is essential. The challenge is that how much stormwater may get into a pond after a storm is very uncertain.

3.8 | Process and supply chain design

3.8.1 | Ecosystems as unit operations

Minimizing the use of Water in the process industries has been an active area of research, which has resulted in methods based on the concept of water pinch and optimization methods to design optimal water networks. Most studies consider only the industrial process as their system boundary. Still, some recent efforts also account for the water footprint or life cycle water use and activities in the watershed.

Recent work by Gopalakrishnan and Bakshi[12] has introduced the idea of considering ecosystems to be unit operations and including them in process design. This work found that including the treatment of wetlands in the process can provide designs that are economically and ecologically superior to conventional technology-centric designs, which is conveyed by the Pareto curve in Figure 11. This figure considers designs with a technological alternative: anaerobic baffled reactor (Pathways 1, 3, 5), and an ecological alternative: treatment of wetland (Pathways 2, 4, 6). These systems are connected to the biodiesel process as an end-of-pipe solution (Pathways 1, 2), as an integrated design with the rest of the flowsheet (Pathways 3, 4), as an integrated design with recycle of the treated Water (Pathways 5, 6). The x-axis is the NPV, and the y-axis is the net water supply in kg/year. The results show that the design with wetlands or TES design is better than the conventional techno-centric design for all three

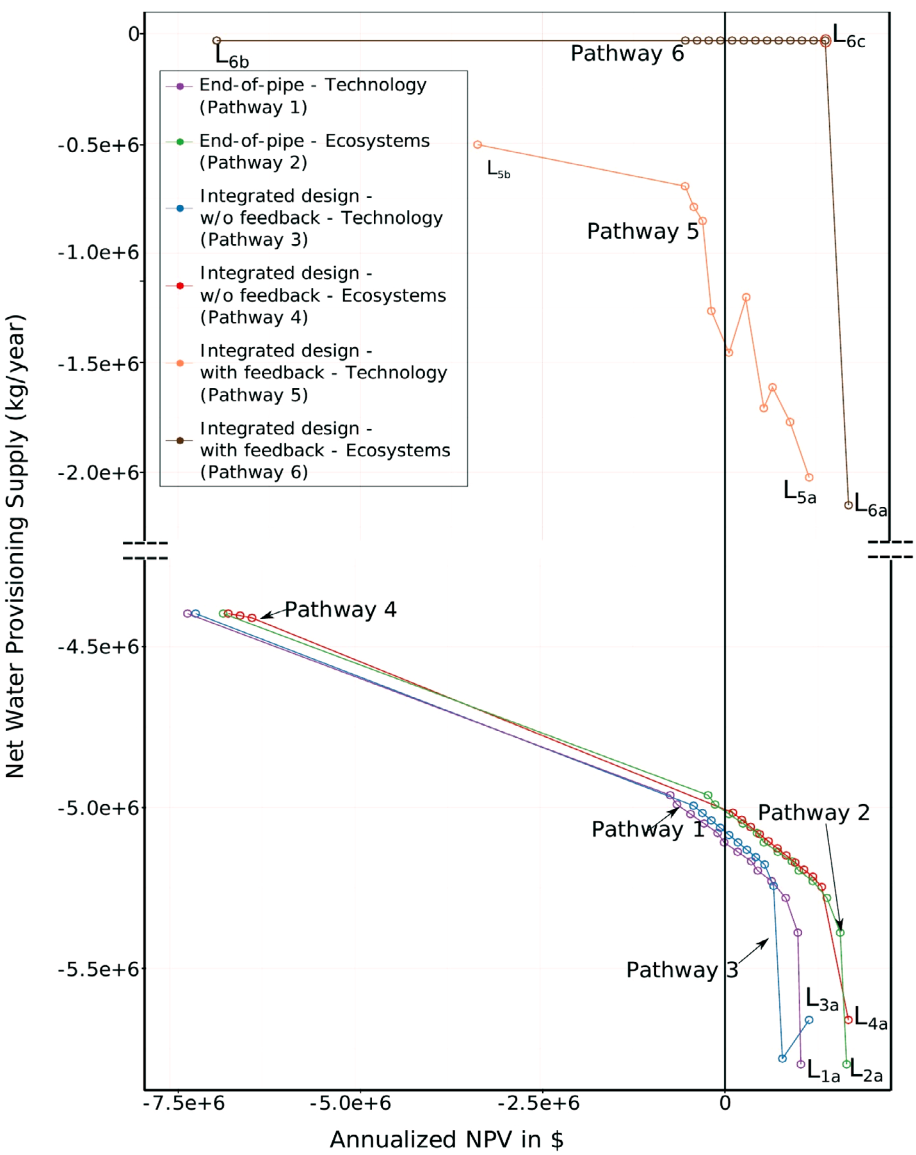

FIGURE 11 Pareto curves for water treatment by anaerobic baffled reactor versus treatment wetland as end-of-pipe, integrated design, and integrated design with water recycling.[41] Reproduced with permission [Color figure can be viewed at wileyonlinelibrary.com]

cases since the Pareto curve for TES is to the left and above the Pareto curve for conventional design. Thus, for the same net water supply, TES design can have a higher NPV than the best conventional design. The integrated design with water recycling is far superior to the other options for the water objective and nearly reaches net-zero Water (Pathway 6). These results demonstrate the potential benefits of including ecosystems as unit operations in process design.

As described by Gopalakrishnan and Bakshi,[12] the integrated designs with wetlands require a different operation of the biodiesel process as compared to conventional designs. Because of the relatively inexpensive separation enabled by the treatment wetland, the integrated design relies less on technologies such as distillation to remove pollutants that could be removed by the wetland. In addition to wetlands, other ecosystems can also play a role in improving water quantity and quality. For example, vegetation that is indigenous to the geographical region can reduce water runoff and help in recharging aquifers. Reducing runoff can also reduce the waste treatment load on the urban infrastructure. Various green infrastructure solutions are available for improving water quality and quantity, including bioswales, buffer strips, and wetlands.

Despite these promising results, more work is needed before the TES designs can be implemented in practice. More case studies are required to gain insight into when ecosystems can perform better than technological systems. In practice, a prudent combination of technical and ecological systems often referred to as “gray” and “green” infrastructure, respectively, is likely to work best. Wetland models are widely available,[42] but may need to be tailored for various compositions of industrial wastes. Implementation of ecosystems in process simulation tools will be required to enable their broad and convenient consideration in process design.

3.8.2 | Spatial supply chains and life cycles

The availability and use of Water vary according to geographical location. A watershed of a lake or river is the region from which precipitation drains into this water body. Thus, from the perspective of water sustainability, a watershed is a self- contained region. If water use in the region does not exceed the availability of renewable Water, the watershed may be considered to be sustainable. Given this insight, decisions involving water use need to take spatial aspects into account at the scale of a watershed. However, a watershed is a complicated system that involves interaction between multiple components such as soil, vegetation, precipitation, water bodies, and human activities. Fortunately, hydrological modeling has been an active area of research, and modeling systems such as the SWAT are available.[25] This model and others described in Section 3.2 need to be used with methods for process design and supply chain management to develop systems that are Water sustainable at the scale of the selected watershed. Depending on the resolution of these models, the resulting optimization problems can be very large, so opportunities may exist for developing and applying advanced methods to improve efficiency. Some steps in this direction are described by Burgara-Montero et al.[43]; Lopez-Diaz et al.[44]; Ghosh and Bakshi.[45] A similar approach may also be used for assessing water sustainability over a life cycle. LCA has been a popular approach to account for the environmental impact from “cradle to grave.” Such a large boundary is used to reduce the chance of burden shifting. For water sustainability, a related approach of water footprint has been developed.[19] Such approaches usually encourage decisions that do less harm by emitting less pollution or using less resources. Such results are useful for comparing alternatives, but they do not give an idea of whether the relevant ecosystem has the capacity to support the activity. Spatial analysis of the life cycle impact or water footprint that accounts for the availability of renewable Water in a watershed is needed to quantify water sustainability of the life cycle. Metrics such as the water scarcity index depicted in Figure 2 account for the supply and demand of Water. Approaches for including the capacity of ecosystems in LCA are also being developed,[46,47] and need to be incorporated in methods for the design of water sustainable processes and supply chains. Furthermore, these larger-scale approaches need to be integrated with process models to incorporate engineering knowledge, and with economic models to account for human behavior and the effect of markets. The process-to-planet framework[48] could be a starting point to enable such integration in a systematic manner.

3.8.3 | Reconciling the dynamics of technological and ecological systems

The behavior of technological and ecological systems is usually vastly different.[17] Technological systems follow the approach of “imposed design,” while ecosystems are “self-designed.” That is, humans design technologies to behave in a very predictable and highly controllable manner to provide a narrow array of services for which they are designed. For example, a light bulb is designed to provide light instantaneously and can be controlled by flipping a switch.

In contrast, ecosystems are much more difficult to predict and provide multiple services but intermittently. For example, a wetland is a self-organized system consisting of many different species that can take weeks or months to develop and grow. During this period, their capacity to provide water quality regulation service is likely to be quite limited. Once established, a wetland can not only provide this service, but can also provide other services such as carbon sequestration, home for biodiversity, and flood regulation. A wetland's behavior can be intermittent due to seasonal variations. Due to these characteristics, thermal energy storage systems may also provide intermittent production, or if this is not acceptable, novel designs and control systems may be needed to obtain predictable behavior while benefiting from synergies between technology and nature.

3.9 | Nexus of water with emissions and resource flows

As discussed in Section 2, to avoid the shifting of environmental problems, water sustainability cannot be isolated, since it is related to other emissions and resource flows. Therefore, methods are needed to understand and account for the nexus between Water, emissions, and resource use. The food-energy-water nexus has received attention, and the potential role of PSE in addressing it has been discussed.[49] Such studies require consideration of the extensive life cycle system, along with the role of ecosystems. Given the large scale of these connections, approaches based on the macroeconomy would be needed to manage the tradeoffs between various flows. Multi-objective optimization methods are certainly relevant, as are methods based on game theory for designing schemes for trading of emissions and ecosystem services,[44] which also requires the development and use of approaches for internalizing costs that are excluded from the market such as those due to pollution. PSE may be able provide the underlying framework for supporting decisions at the interface of the economy, environment, and industry.

4 | CONCLUDING REMARKS

Water is essential for the sustainability of our society. We are facing significant challenges of insufficient water quantity and poor water quality, and these challenges are expected to become worse due to a combination of an increasing population, more prosperity, and climate change. A systems view is vital in addressing these challenges, and this presents many opportunities and challenges for PSE. Agriculture is the largest consumer of freshwater, and the current agriculture irrigation is essentially in *open loop*. To close the loop in agriculture irrigation decision making, there are many significant challenges in agro-hydrological systems modeling, sensing, and water management. To meet the goals of water sustainability, the boundary of traditional PSE should be expanded to incorporate ecosystems, and new process design and assessment methods should be developed. In addition, nature's capacity to supply goods and services should be respected. Address these challenges requires PSE researchers to work closely with researchers and practitioners in multiple disciplines, including agriculture, ecology, hydrology, environmental engineering, soil science, and computer science.

ACKNOWLEDGMENTS

The first and third authors gratefully acknowledge help from Soumya Sahoo of the University of Alberta for the many comments and suggestions in the early draft of this manuscript.

ORCID

Bhavik R. Bakshi https://orcid.org/0000-0002-6604-8408
Jinfeng Liu https://orcid.org/0000-0001-8873-847X
Christos Georgakis https://orcid.org/0000-0001-9895-8564

REFERENCES

1. UN Water. World water development report—water for a sustainable world. United Nations; 2015.
2. World Economic Forum. Global risks 2015. 10th ed.; 2015.
3. World Economic Forum. The global risks report 2019. 14th ed.; 2019.
4. FAO. AQUASTAT website. Food and Agriculture Organization of the United Nations (FAO); 2016.
5. Breitburg D, Levin LA, Oschlies A, et al. Declining oxygen in the global ocean and coastal waters. *Science*. 2018;359(6371):eaam7240.
6. Foo DCY. State-of-the-art review of pinch analysis techniques for water network synthesis. *Ind Eng Chem Res*. 2009;48(11):5125-5159.
7. European Environment Agency. Use of freshwater resources; 2018.
8. State Council of China. Regulations of irrigation and water conservancy; 2016.
9. United States Department of Agriculture. Irrigation & water use. https://www.ers.usda.gov/topics/farm-practices-management/irrigation-water-use. Accessed September 4, 2019.
10. FAO. Climate change, water and food security. Food and Agriculture Organization of the United Nations (FAO); 2008.
11. UN Water. World water development report—water in a changing world. United Nations; 2009.
12. Bakshi BR, Gutowshi TG, Sekulic DP. Claiming sustainability: requirements and challenges. *ACS Sustain Chem Eng*. 2018;6(3):3632-3639.
13. Azapagic A, Clift R. Life cycle assessment and linear programming environmental optimization of product system. *Comput Chem Eng*. 1995;19(Suppl):229-234.
14. Grossmann IE. Challenges in the new millennium: product discovery and design, enterprise and supply chain optimization, global life cycle assessment. *Comput Chem Eng*. 2004;29(1):29-39.
15. Stefanis SK, Livingston AG, Pistikopoulos EN. Minimizing the environmental impact of process plants: a process systems methodology. *Comput Chem Eng*. 1995;19(Suppl):39-44.
16. Bakshi BR. *Toward* sustainable chemical engineering: the role of process systems engineering. *Annu Rev Chem Biomol Eng*. 2019;10:265-288.
17. Bakshi BR, Ziv G, Lepech MD. Techno-ecological synergy: a framework for sustainable engineering. *Environ Sci Technol*. 2015;49(3):1752-1760.
18. Interdisciplinary Research Team Summaries the National Academies Keck Futures Initiative. *Ecosystem services: charting a path to sustainability*. Washington, DC: National Academies Press; 2012.
19. Hoekstra AY. *The water footprint of modern consumer society*. London, UK: Routledge; 2013.
20. Ferrandez-Villena M, Ruiz-Canales A, eds. Advances on ICTs for water management in agriculture. Special Issue of Agricultural Water Management; 2017.
21. United States Geological Survey. Irrigation water use: surface irrigation. https://water.usgs.gov/edu/irfurrow.html. Accesed June 11, 2018.
22. Richards LA. Capillary conduction of liquids through porous mediums. *J Appl Phys*. 1931;1:318-333.
23. Allen RG, Pereira LS, Raes D, Smith M. FAO irrigation and drainage paper. Technical Report 56, Food and Agriculture Organization of the United Nations; 1998.
24. Mayne DQ, Rawlings JB, Rao CV, Scokaert POM. Constrained model predictive control: stability and optimality. *Automatica*. 2000;36:789-814.
25. Douglas-Mankin KR, Srinivasan R, Arnold JG. Soil and water assessment tool (SWAT) model: current developments and applications. *Trans ASABE*. 2010;53:1423-1431.
26. Steduto P, Hsiao TC, Raes D, Fereres E. AquaCrop—the FAO crop model to simulate yield response to water: I. concepts and underlying principles. *Agron J*. 2009;101:426-437.
27. Vanclooster M, Viaene P, Diels J. WAVE: A mathematical model for simulating Water and agrochemicals in the soil and vadose environment (release 2.0). Technical Report, Katholieke Universiteit Leuven; 1994.
28. Petropoulos GP, Ireland G, Barrett B. Surface soil moisture retrievals from remote sensing: current status, products & future trends. *Phys Chem Earth*. 2015;83–84:36-56.

29. De Lannoy GJM, Houser PR, Pauwels VRN, Verhoest NEC. State and bias estimation for soil moisture profiles by an ensemble Kalman filter: effect of assimilation depth and frequency. *Water Resour Res*. 2007;43:W06401.
30. Nahar J, Liu J, Shah SL. Parameter and state estimation of an agro-hydrological system based on system observability analysis. *Comput Chem Eng*. 2019;121:450-464.
31. Sahoo SR, Yin X, Liu J. Optimal sensor placement for agro-hydrological systems. *AICHE J*. 2019;65:1-18.
32. Belayneh BE, Lea-Cox JD, Lichtenberg E. Costs and benefits of implementing sensor- controlled irrigation in a commercial pot-in-pot container nursery. *HortTechnology*. 2013;23:760-769.
33. Gutierrez J, Villa-Medina JF, Nieto-Garibay A, Porta-Gandara MA. Automated irrigation system using a wireless sensor network and GPRS module. *IEEE Trans Instrum Meas*. 2014; 63:166-176.
34. Saavoss M, Majsztrik J, Belayneh B, Lea-Cox J, Lichtenberg E. Yield, quality and profitability of sensor-controlled irrigation: a case study of snapdragon production. *Irrig Sci*. 2016;34:409-420.
35. Antoulas AC. *Approximation of Large-Scale Dynamical Systems*. New York, NY: SIAM Press; 2005.
36. Xie W, Bonis I, Theodoropoulos C. Off-line model reduction for on-line linear MPC of nonlinear large-scale distributed systems. *Comput Chem Eng*. 2011;35:750-757.
37. Mao Y, Liu S, Nahar J, Liu J, Ding F. Soil moisture regulation of agro-hydrological systems using zone model predictive control. *Comput Electron Agric*. 2018;154:239-247.
38. Christofides PD, Scattolini R, Munoz de la Pena D, Liu J. Distributed model predictive control: a tutorial review and future research directions. *Comput Chem Eng*. 2013;23:404-414.
39. Milesi C, Elvidge CD, Nemani RR. Assessing the extent of urban irrigated areas in the United States. *Remote Sensing of Global Croplands for Food Security*. Boca Raton, FL: CRC Press, Taylor & Francis Group; 2009:217-236 (Chapter 8).
40. Nahar J, Liu S, Liu J, Shah SL. Improved storm water management through irrigation rescheduling for city parks. *Control Eng Pract*. 2019; 87:111-121.
41. Gopalakrishnan V, Bakshi BR. Ecosystems as unit operations for local techno-ecological synergy: integrated process design with treatment wetlands. *AICHE J*. 2018;64(7):2390-2407.
42. Kadlec RH, Wallace SD. *Treatment wetlands*. 2nd ed. Boca Raton, FL: CRC Press; 2009.
43. Burgara-Montero O, Ponce-Ortega JM, Serna-Gonzalez M, El-Halwagi MM. Incorporation of the seasonal variations in the optimal treatment of industrial effluents discharged to watersheds. *Ind Eng Chem Res*. 2013;52(14):5145-5160.
44. Lopez-Diaz DC, Lira-Barragan LF, Rubio-Castro E, Ponce-Ortega JM, El-Halwagi MM. Synthesis of eco-industrial parks interacting with a surrounding watershed. *ACS Sustain Chem Eng*. 2015;3(7):1564-1578.
45. Ghosh T, Bakshi BR. Designing biofuel supply chains while mitigating harmful algal blooms with treatment wetlands. *Comput Chem Eng*. 2019;126:113-127.
46. Boulay AM, Bare J, Benini L, et al. The WULCA consensus characterization model for water scarcity footprints: assessing impacts of water consumption based on available water remaining (AWARE). *Int J Life Cycle Assess*. 2018;23(2):368-378.
47. Liu X, Bakshi BR. Ecosystem services in life cycle assessment while encouraging techno- ecological synergies. *J Ind Ecol*. 2019;23(2): 347-360.
48. Hanes RJ, Bakshi BR. Process to planet: a multiscale modeling framework toward sustainable engineering. *AICHE J*. 2015;61(10):3332-3352.
49. Garcia DJ, You F. The water-energy-food nexus and process systems engineering: a new focus. *Comput Chem Eng*. 2016;91:49-67. ISSN 0098-1354.

How to cite this article: Shah SL, Bakshi BR, Liu J, et al. Meeting the challenge of water sustainability: The role of process systems engineering. *AIChE J*. 2021;67:e17113. https://doi.org/10.1002/aic.17113