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Key Points:

- Review opportunities to apply ecohydrology methods in agroecosystems
- Parsimonious models address stochasticity and nonlinearity in ecohydrology
- Sustainable soil and water use can be designed via optimal stochastic control

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Ecohydrological modeling in agroecosystems: Examples and challenges

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Abstract Human societies are increasingly altering the water and biogeochemical cycles to both improve ecosystem productivity and reduce risks associated with the unpredictable variability of climatic drivers. These alterations, however, often cause large negative environmental consequences, raising the question as to how societies can ensure a sustainable use of natural resources for the future. Here we discuss how ecohydrological modeling may address these broad questions with special attention to agroecosystems. The challenges related to modeling the two-way interaction between society and environment are illustrated by means of a dynamical model in which soil and water quality supports the growth of human society but is also degraded by excessive pressure, leading to critical transitions and sustained societal growth-collapse cycles. We then focus on the coupled dynamics of soil water and solutes (nutrients or contaminants), emphasizing the modeling challenges, presented by the strong nonlinearities in the soil and plant system and the unpredictable hydroclimatic forcing, that need to be overcome to quantitatively analyze problems of soil water sustainability in both natural and agricultural ecosystems. We discuss applications of this framework to problems of irrigation, soil salinization, and fertilization and emphasize how optimal solutions for large-scale, long-term planning of soil and water resources in agroecosystems under uncertainty could be provided by methods from stochastic control, informed by physically and mathematically sound descriptions of ecohydrological and biogeochemical interactions.

1. Ecohydrology: From Natural to Managed Ecosystems

"Ecohydrology may be defined as the science which seeks to describe the hydrologic mechanisms that underlie ecologic patterns and processes" [*Rodriguez-Iturbe*, 2000]. These mechanisms are ubiquitous and centered on the deep relation between vegetation, soil microbes, and soil water [*Cowan*, 1986; *Rodríguez-Iturbe and Porporato*, 2004]. Such interactions tend to be most compelling in semiarid ecosystems, where the availability of water (or lack thereof) plays a strong role in ecosystem processes, but extend to any interaction between biota and water in both terrestrial and aquatic ecosystems [e.g., *Eagleson*, 2002; *Lohse et al.*, 2009; *Manzoni and Porporato*, 2009, 2011; *Newman et al.*, 2006; *Ridolfi et al.*, 2011, among many others].

One key aspect of ecohydrological processes is the variability and unpredictability of the hydrologic drivers and, consequently, of water availability. Methods of stochastic ecohydrology have quantitatively addressed this unpredictability, by treating the hydroclimatic forcing of ecohydrological systems as random functions and thus allowing for probabilistic analyses of the propagation of such variability through different processes within the systems [*Ridolfi et al.*, 2011; *Rodríguez-Iturbe and Porporato*, 2004]. This variability, especially through the impacts of droughts and floods on safety and food security, not only impacts natural ecosystems but has historically been an important modulator of social and economic systems, triggering phases of social growth and collapse. *Verchuren et al.* [2000] offer an interesting example where drought-related political upheavals recorded in East African oral tradition occurred often during periods of low water availability.

Humans have spent increasingly large efforts to reduce the volatility of water resource availability and defend themselves from natural hazards [*Vörösmarty et al.*, 2010]. We have improved the rate of extraction of food and fiber from ecosystems by managing vegetation, engineering landscapes, soils, and drainage systems and by intensely controlling the quantity and quality of water, carbon, and nutrient fluxes in and out of ecosystems [*Haberl et al*., 2007; *Rojstaczer et al*., 2001; *Vitousek et al*., 1997], resulting in increasingly stronger human feedbacks on the hydrosphere and ecosystems. This coupling of human and ecohydrological systems is particularly strong in agricultural systems and parallels that between plants and the hydrologic cycle in natural ecosystems, where plants are impacted by and, in turn, impact the hydrologic cycle [*Rodríguez-Iturbe and Porporato*, 2004]: "Man and water are closely related to each other in a dualistic manner," because "On one hand, [man] is deeply dependent on water not only for his survival but for numerous functions of society. . . .On the other hand, this dependence forces man to intervene in numerous ways with the natural water circulation system" [*Falkenmark*, 1979].

Ecohydrology-based methods may offer environmentally informed solutions to sustainable development of agricultural systems, which are often highly degraded but have the potential to provide valuable ecosystem services [*Altieri*, 1999]. These theories may provide guidelines for sustainable use of soil and water resources from a different angle compared to classical agronomic and ecological approaches [*Newman et al*., 2006; *Porporato and Rodriguez-Iturbe*, 2002]. Beyond applications in agroecosystems, they can also be applied in urban environments [*Pataki et al*., 2011], and to address biota-water interactions in streams and wetlands [*Kundzewicz*, 2002; *Muneepeerakul et al*., 2007; *Tamea et al*., 2010; *Todd et al*., 2012]. We have chosen a relatively narrow focus within this vast subject, concentrating on specific examples related to our own research to emphasize the importance of a minimal-complexity, stochastic approach and to illustrate some of the challenges that this entails. We hope to be forgiven for having left aside many other areas (even within agroecosystem research) that, although interesting and valuable, would have taken us too far, and wish that the imaginative readers will anyhow find some useful suggestions for their own specific research. For example, while it is almost immediate to extend the existing results of ecohydrology to quantify productivity and water stress in the important context of rainfed agriculture, these issues will not be discussed here.

The paper is organized as follows. In section 2, we discuss how ecosystem management accelerates water and biogeochemical cycling, increases the fragility of ecosystems, and may ultimately lead to ecosystem collapse. This process is conceptualized as a nonlinear dynamical system coupling human and ecosystem dynamics, which provides a macroscopic view of the possible management outcomes. Section 3 presents a quantitative framework to address nonlinear, stochastic dynamics in soil-plant systems. This framework is then applied to irrigated agroecosystems, fertilization, and soil degradation, and remediation. In section 4, we argue that each of these management challenges involve the control/alteration of coupled water and nutrient/contaminant fluxes and can be framed as optimal stochastic control problems. Finally, in section 5, we draw conclusions and outline directions for future research.

2. Acceleration of Water and Biogeochemical Cycles and Degradation of Ecosystem Quality: A Modeling Challenge

Ecosystems may be seen as open thermodynamics systems that exchange mass, energy, and entropy in nonequilibrium conditions [*Jørgensen and Svirezhev*, 2004]. Through inputs from solar radiation and water, carbon, and nutrient fluxes, ecosystems build and store organic compounds with high energy availability (i.e., chemical potential) that are used for the growth, maintenance, and reproduction of their constituent members. Human management of water and biogeochemical cycles increases productivity, accelerates internal cycling of water, energy, and nutrients (Figure 1)—as is the case for irrigation and fertilization—albeit often at the expense of biodiversity, resilience, and other ecosystem services [*Altieri*, 1999; *Lin*, 2011]. Thus, despite increased productivity, the very efforts to stabilize ecosystem response to small environmental fluctuations may cause over-specialization, over-exploitation, and hence a loss of redundancy, which in turn may increase vulnerability to extreme fluctuations [*Scheffer et al*., 2001]. These systems become then unable to provide essential ecosystem services, resulting in reduced environmental quality and stability and potentially moving closer to possible tipping points and catastrophic thresholds [*Altieri*, 1999; *Barnosky et al*., 2012].

Dramatic examples of such regime shifts range from large-scale irrigation and deforestation that triggered loss of fertile land due to erosion and salinization [*Hillel*, 1998], to desertification induced by land over-exploitation [*Reynolds et al*., 2007]. In arid ecosystems, vegetation engineers its environment by creating soil for water storage to maintain the water supply necessary to support physiological activity and growth.

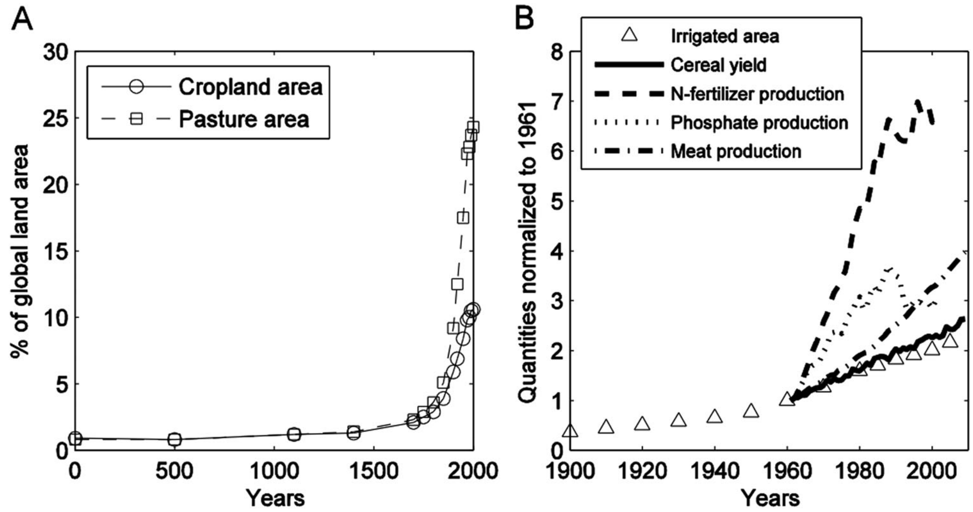

Figure 1. (a) Increased human pressure on land in the last two millennia [*Goldewijk et al*., 2011], and (b) acceleration of biogeochemical cycles by agricultural intensification (in terms of cereal yield, irrigated land, fertilization, and meat production) in the last century (irrigated land data from *Siebert et al*. [2015]; other data from FAO).

Once vegetation is degraded, this positive feedback is destabilized, causing a shift to a nonvegetated state [*Cook et al*., 2009; *Konings et al*., 2011; *Reynolds et al*., 2007; *Runyan et al*., 2012; *Scheffer et al*., 2001; *Zelnik et al*., 2013]. The risk of such shifts can be intensified by severe drought or other temporary lack of resources, such as during the 1930s Dust Bowl in the USA (Figure 2). As exemplified by the establishment of the Soil Conservation Service and other emergency relief efforts following the Dust Bowl, substantial resource investments are often required to revert degraded landscapes to their prior productive state.

Most existing models exploring the role of feedbacks in desertification and land degradation treat human influence as external to the ecosystem. A conceptual model of interacting natural and human-driven agricultural ecosystems may be useful here to illustrate the qualitative changes induced by these interactions.

Consider a total land area, A, partitioned between managed agricultural land area, A_{ag}, yielding food and economic benefits to the population, and natural land area, $A_{nat}=A-A_{ag}$, which yields associated ecosystem services. In this framework, A_{ag} is a proxy for social dynamics—increasing A_{ag} indicates a developing social system, whereas decreasing A_{ag} mirrors a declining society. A dynamic "ecosystem quality" q (with unspecified units q), that aggregates the effects of ecosystem degradation by agricultural development and ecosystem renewal through natural processes, is sustained by the system ability to provide ecosystem services η (q yr^{-1}) (i.e., healthy ecosystems provide more services, which in turn increase their quality) and is bounded by a nonlinear function that ensures a steady state for a given level of ecosystem services. The corresponding dynamic equation for q reads,

$$\frac{dq}{dt}=\eta-c\left(\frac{q}{q_0}\right)^{\alpha}, \tag{1}$$

where the rate of turnover c (q yr^{-1}) and the exponent α control both the equilibrium value, $q^*=q_0(\eta/c)^{1/(\alpha+1)}$, and how quickly q approaches it. In what follows the reference quality, q_0, is assumed equal to 1 and α is assumed equal to 2.

Ecosystem services provided by the environment η may be assumed to depend on three factors: (i) external inputs from surrounding areas, η_0 (q yr^{-1}), a measure of nonisolation; (ii) the extent of the natural land area and the quality of the environment; and (iii) negative impacts from adjacent agricultural activities (e.g., nutrient runoff, reduction of biodiversity, etc.),

$$\eta=\eta_0+k_{nat}q\,A_{nat}-k_{ag}A_{ag}, \tag{2}$$

where k_{nat} (ha^{-1} yr^{-1}) converts quality to ecosystem services and k_{ag} (q ha^{-1} yr^{-1}) is the degradation rate resulting from nearby agricultural practices.

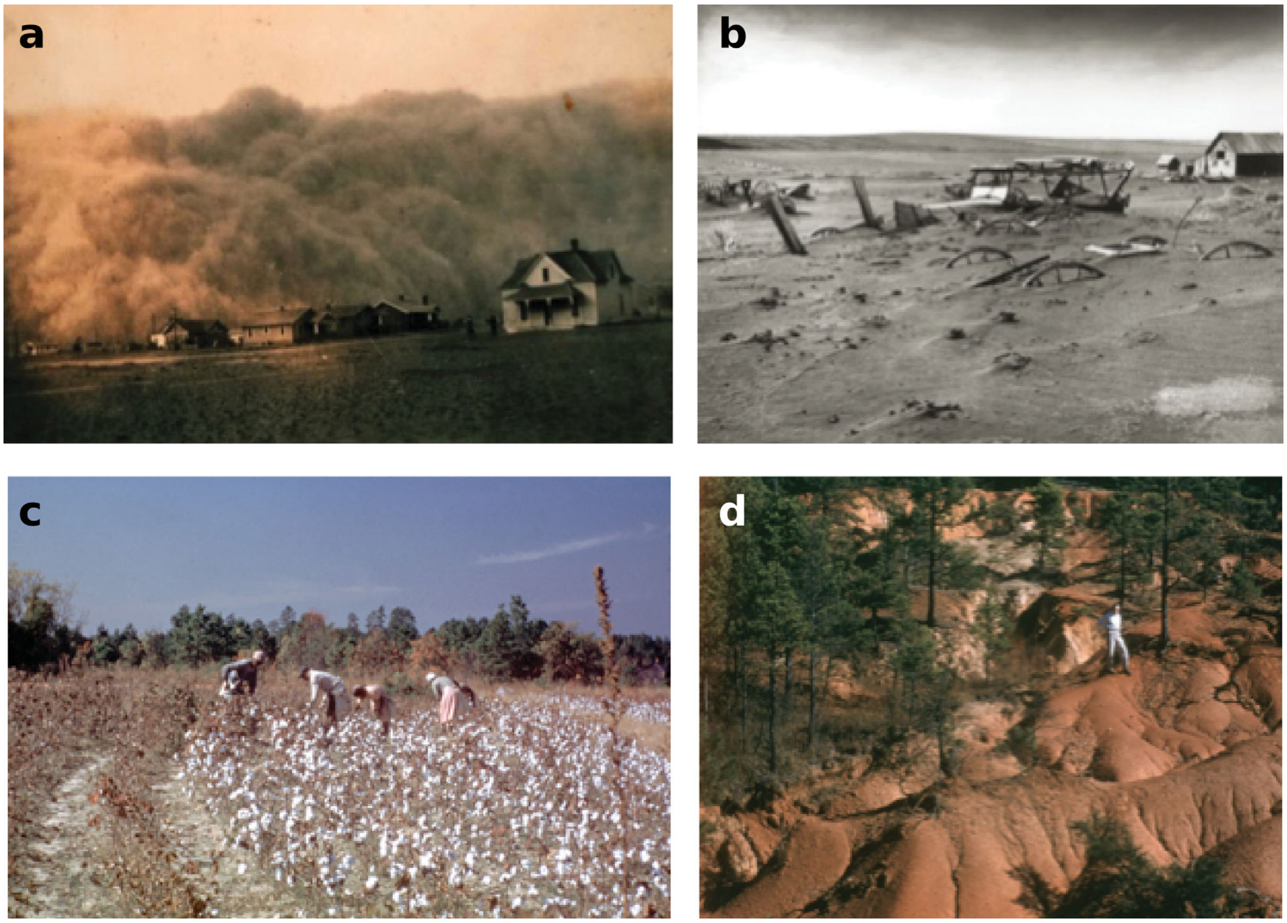

Figure 2. Examples of catastrophic soil loss under intensive land use pervade the agricultural history of the United States. The 1930s Dust Bowl was in part accelerated by severe drought, as described by John Steinbeck, whose literary work documented the environmental and economic disaster that eventually displaced hundreds of thousands of Great Plains farmers, "*Little by little the sky was darkened by the mixing dust, and the wind felt over the earth, loosened the dust, and carried it away. The wind grew stronger*" [*Steinbeck*, 1939]. (a) Dust storm approaching Stratford, Texas, 18 April 1935. (b) Buried machinery in a barn lot in Dallas, South Dakota, May 1936. Much of the southeastern U.S. experienced agricultural degradation due to accelerated water erosion initiated in the nineteenth century with the expansion of cotton. According to Fisk University Professor Charles S. Johnson, the cotton-producing South in the 1930s was "*a miserable panorama of unpainted shacks, rain-gullied fields, straggling fences, and rattletrap Fords, dirt, poverty, disease, . . . and monotony that stretches for a thousand miles across the cotton belt*" [*Johnson et al*., 1935]. (c) Thousands of farm families, mostly debt-ridden tenants and share croppers, cultivated cotton with mule and plow and much hand labor. (d) Widespread erosion accompanied cultivation, eventually resulting in substantial losses of surface soils and severe gullying, greatly reducing the land's native productivity. Photo credits: (a) NOAA George E. Marsh Album, (b) U.S. Department of Agriculture, (c and d) USDA Forest Service at Calhoun Critical Zone Observatory (http://criticalzone.org/calhoun/).

The other state variable in this system, the managed agricultural land area, A_{ag}, is assumed to increase with environmental quality, as the associated food and economic benefits of production stimulates human interest in cultivating more land. In addition, we allow for the influence of external markets to drive land cultivation within the system at a rate A_0 (ha yr^{-1}), another measure of nonisolation. We introduce an additional term to ensure that A_{ag} does not exceed the total land area, A. With these assumptions the temporal evolution of the agricultural area can be described as,

$$\frac{dA_{ag}}{dt}=\left(k_h q A_{ag}+A_0\right)\left(1-\frac{A_{ag}}{A}\right), \tag{3}$$

where k_h (q^{-1} yr^{-1}) is the rate at which agricultural land is developed in response to the benefits of production. Equations (1–3) comprise a two-dimensional dynamical system for coupled agricultural area and environmental quality.

The previous dynamical system describes a feedback between agricultural area and environmental quality that involves the negative influence of increased human pressure on ecosystem services and, thus, agricultural productivity. Expanding human pressure to larger areas decreases the quality of natural ecosystems,

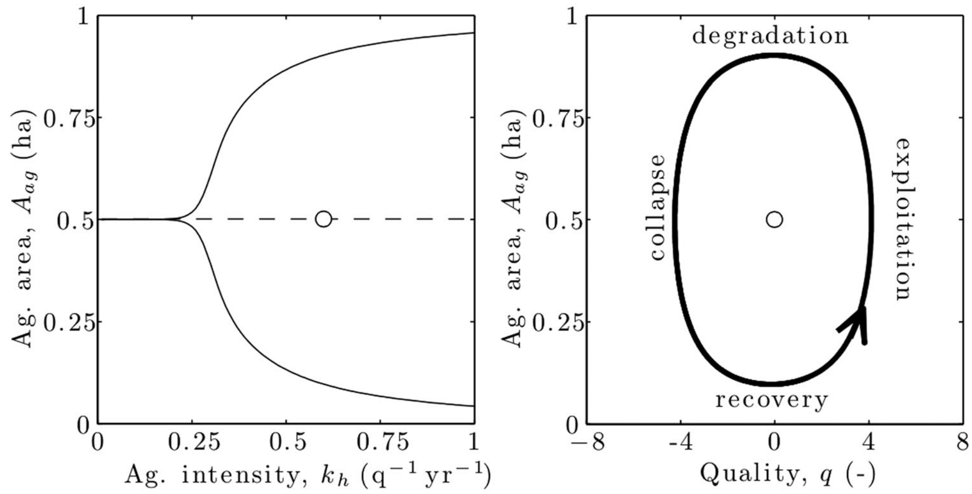

Figure 3. Dynamics of the coupled human-natural system described in section 2. (left) Bifurcation diagram for agricultural area as a function of the control parameter, k_h, which represents the intensity with which the social system responds to the benefits of land cultivation. The system undergoes a supercritical Hopf bifurcation from a single, stable fixed point, approached through decaying spirals, to a stable limit cycle that surrounds an unstable fixed point. (right) System trajectory plotted in the quality-agricultural area phase space for the limit cycle regime. Solid lines depict stable points (or limit cycle), the dashed lines depict unstable points, and the open circle depicts the unstable fixed point. Parameter values used for the coupled human-environment system are $A=10^5$ ha, $A_0=10^3$ ha yr^{-1}, $k_{nat}=4.88\times10^{-4}$ m^{-2} yr^{-1}, $\eta_0=5$ q yr^{-1}, $c=10^{-3}$ q^{-1} yr^{-1}, $k_{ag}=10^{-4}$ q ha^{-1} yr^{-1}.

which in turn inhibits productivity and further growth, and thereby provides a stabilizing mechanism (i.e., a system carrying capacity). The presence of an interaction term (qA_{ag}) makes this dynamical system prone to bifurcations as a function of the control parameter k_h (Figure 3), which controls the rate at which agricultural development responds to environmental quality and existing agricultural productivity, i.e., the current food and economic output of the land. As the social system responds more rapidly to agricultural production (i.e., higher k_h), the system shifts from that characterized by a single, stable, and productive fixed point approached through decaying spirals to a limit cycle that oscillates between productive and degraded states. This bifurcation is a supercritical Hopf bifurcation, characterized by a loss of stability at the critical point [*Argyris et al*., 1994; *Strogatz*, 2014].

As the social system becomes more sensitive to agricultural production and ecosystem quality (i.e., increasing k_h), its limit cycle dynamics can be described as a self-sustaining sequence of four phases: exploitation, degradation, collapse, and recovery (Figure 3b). In the exploitation phase, environmental quality is constantly high and agricultural area expands rapidly. Subsequently, the natural environment is degraded during a period of consistent intensive land use. Once the quality has decreased to a sufficient level, agricultural pressure is released in the collapse phase, either through the implementation of conservation practices or due to severe resource impairment. With the release of agricultural pressure, the natural ecosystem then recovers and the system reenters the exploitation phase. This sequence of phases is conceptually similar to the exploitation-conservation-release-reorganization paradigm introduced by *Holling* [2001].

The coupled system of equations (1–3) extends the previously proposed bistable systems approach [e.g., *Scheffer et al*., 2001; *Runyan et al*., 2012]. In this coupled social-ecological system framework, the exploitation and collapse phases dynamically link the bistable vegetated and nonvegetated states described in previous work, which correspond to the degradation and recovery phases, respectively. The challenge, however, is to embed these human actions on the environment at a more fundamental and basic level so that quantitative models become capable of predicting the time scales and risk of approach to such catastrophic thresholds [*Kéfi et al*., 2013; *Sornette*, 2002] and the system responses to human decisions [*Carpenter et al*., 2009; *Parolari et al*., 2015; *Van Emmerik et al*., 2014]. Such models will necessarily need to balance the representation of the complexity in the environment (due to stochastic forcing and many degrees of freedom in the soil-plant spatially extended system) with the complexity of human decision-making and risk perception [e.g., *An*, 2012; *Baldassarre et al*., 2013; *Lehmann et al*., 2013].

3. The Challenge of Stochastic Forcing and Nonlinear Interactions

Ecohydrological processes are often strongly nonlinear—a fact that amplifies the intermittency and unpredictability of the external hydroclimatic fluctuations that drive them. Thus, a framework that blends process-based representations of ecohydrological and biogeochemical dynamics, nonlinearities, and random components of the forcing is necessary to tackle the problem of sustainable management of water, soil, and ecosystem resources in a quantitative way. Along these lines, the methods developed by stochastic ecohydrology [*Rodríguez-Iturbe and Porporato*, 2004] focus on nonlinear interactions and temporal stochasticity, while smoothing out spatial heterogeneities through spatially lumped representations. In this manner, one hopes to achieve predictions that are robust to parameter uncertainties and are easily transferable to future climatic conditions. While such simplifications of the spatial scale hold well in natural ecosystems over larger areas, they are expected to perform even better in an agricultural context, thanks to soil and land homogenization via ploughing, terracing and grading, drainage, etc.

As a starting point, it is logical to choose the coupled balance equations for the mass of water and nutrients/contaminants, open to natural and anthropogenic inputs and outputs and subject to stochastic environmental fluctuations (Figure 4). For simplicity, we will refer to spatially lumped equations describing the vertically averaged dynamics of soil water and solute content over a representative soil rooting zone of depth Z_r of a homogeneous soil of porosity n, with negligible topographic effects (i.e., no significant lateral water redistribution). Vertically averaged approaches have been advocated [*Moore et al*., 2004] for their parsimony, which allows a direct analysis of the interplay of the main processes, and provides an ideal starting point to include external, random hydroclimatic fluctuations in the analyses of soil water and solutes. With these assumptions, the temporal evolution of the relative soil moisture ($0 < s \leq 1$) can be written as [*Rodríguez-Iturbe and Porporato*, 2004]:

$$nZ_r \frac{ds(t)}{dt} = R(t) + I(s(t)) - T(t, s(t)) - L(t, s(t)), \tag{4}$$

where $R(t)$ is the rainfall rate (minus canopy interception), $I(s(t))$ is the irrigation rate, $T(t, s(t))$ combines the rates of soil water evaporation and the plant transpiration, and $L(t, s(t))$ includes both percolation and runoff loss rates as well as capillary rise from the water table.

As in previous ecohydrological models [e.g., *Rodríguez-Iturbe and Porporato*, 2004], the physical interpretation of the processes is at the daily time scale, assuming that all subdaily variability has been averaged out in defining the daily fluxes in equation (4). For a given vegetation cover, the losses by evapotranspiration are controlled by atmospheric water demand, which sets the maximum transpiration under well-watered conditions, and by soil moisture, which reduces transpiration through stomatal closure and reductions in plant and soil-to-root hydraulic conductivities as the soil dries [*Rodríguez-Iturbe and Porporato*, 2004; *Vico and Porporato*, 2008]. At the daily level, rainfall events may be assumed to occur according to a marked Poisson process, with mean frequency of events λ, and with exponentially distributed event depths, with mean depth α [*Rodriguez-Iturbe et al*., 1999]. These parameters may be time dependent to include the effect of seasonality [*Feng et al*., 2012, 2015]. In agricultural systems, an additional input of water through irrigation, I, may be present [*Vico and Porporato*, 2010, 2011a]. In turn, such water input may carry dissolved salts, nutrients, and other compounds [*Assouline et al*., 2006; *Botter et al*., 2008].

The dynamics of dissolved salts, nutrients, or contaminants in the soil is coupled with those of soil water, which affect the solute concentration through plant uptake, leaching, and volatilization. The temporal evolution of the solute mass, m, dissolved in the soil solution per unit area of soil for a generic solute M, can be described by the following mass balance equation:

$$\frac{dm(t)}{dt} = I_n(t) + I_a(t) - \phi(t, s(t)) - U(t, s(t), m(t)) - P(t, s(t), m(t)) - V(t, s(t), m(t)). \tag{5}$$

Here $I_n(t)$ is the rate of natural input by dry and wet deposition, $I_a(t)$ is the anthropogenic input rate, $\phi(t, s(t))$ is the net exchange between soluble and insoluble fractions (e.g., nutrient mineralization from organic matter; adsorption/desorption; dissolution of salts), $U(t, s(t), m(t))$ is the rate of nutrient/contaminant uptake by plants (linked in part to transpiration T in equation (4)), $P(t, s(t), m(t))$ is the rate of solute loss due to leaching and runoff (associated with L), and $V(t, s(t), m(t))$ is the volatilization flux. These generic terms take on specific forms depending on the type of solute analyzed, as detailed in section 3.2.

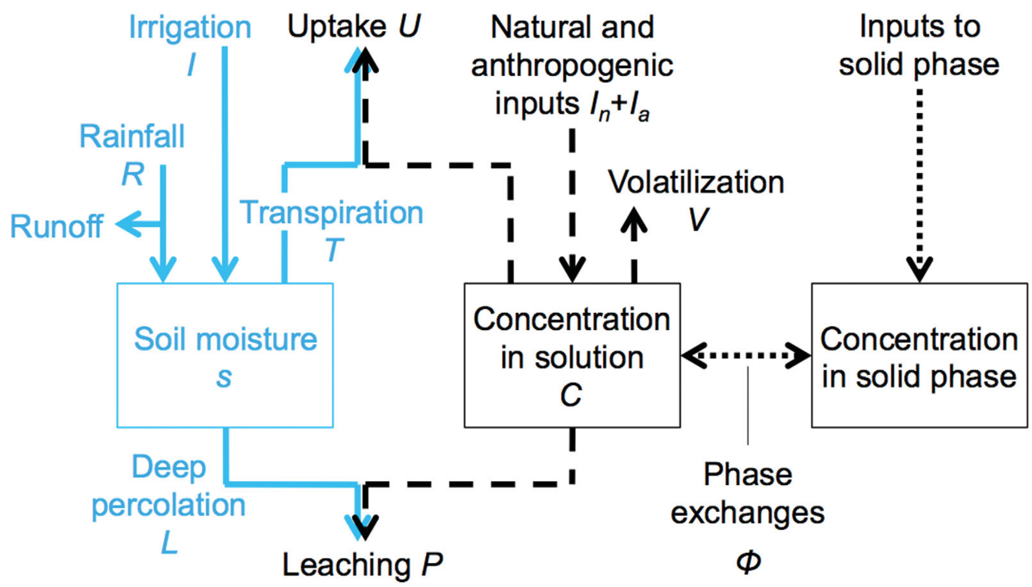

Figure 4. Schematic illustration of mass balances of soil moisture, s, and a generic soil compound in solution with concentration $C=m/(nZ_rs)$ (e.g., nitrate, the soluble fraction of a contaminant, and dissolved salts). Solid lines represent fluxes of water, dashed lines fluxes of dissolved m, and dotted lines fluxes exchanged with adsorbed phase. Equations (4) and (5) describe mathematically this coupled system, forced by natural stochastic rainfall and anthropogenic inputs.

3.1. Stochastic Irrigation

Water demand for irrigation is projected to increase as a result of population growth, changing food habits and biofuel production, and projected climate change [*de Fraiture et al.*, 2010; *Jury and Vaux*, 2007; *Schmidhuber and Tubiello*, 2007]. In addition to the implications related to potential soil salinization (see section 3.2.1) [*Assouline et al.*, 2015], water management through irrigation has also profound implications on river flows and related ecosystem services [*Baron et al.*, 2002; *Eheart and Tornil*, 1999; *Falkenmark and Lannerstad*, 2005; *Miles et al.*, 2006; *Molle et al.*, 2007] as well as groundwater levels and quality [*Caylor et al.*, 2009; *McGuire*, 2009; *Scanlon et al.*, 2007; *Schoups et al.*, 2005].

Despite the key role of rainfall unpredictability on crop yields, research on irrigation optimization has often neglected the effects of daily hydroclimatic variability and the associated economic risks [*English*, 1981; *Oweis and Hachum*, 2009; *Sepaskhah et al.*, 2006] and has instead focused on either long-term scenarios with simplified climatic forcing or on short-term irrigation analyses based on detailed soil-plant models but without inclusion of rainfall stochasticity. The relatively few studies that account for the unpredictability of the climatic conditions are based on simulations with different realizations of the climatic forcing [e.g., see *Mannocchi and Mecarelli*, 1994; *Lehmann et al.*, 2013], stochastic dynamic programming [e.g., *Grafton et al.*, 2011; *Matanga and Marino*, 1979], or genetic algorithms [e.g., *Kumar et al.*, 2006]. All these methods rely heavily on computationally intensive numerical simulations.

The soil moisture balance in equation (4) with stochastic rainfall inputs has been studied to explore the effects of irrigation strategy on productivity, profitability, and sustainability under uncertain climatic conditions [*Vico and Porporato*, 2011b, 2013]. The focus is on demand-based irrigation, in which a water application is triggered by plant or soil water status reaching a preset threshold. Depending on the set level of plant or soil water status at which an irrigation application is initiated, either stress-avoidance or deficit irrigation may be performed. In the first case, the crop is always maintained under well-watered conditions, while the latter case allows a certain level of water stress to occur. As such, deficit irrigation may result in lower water requirements at the cost of yield reduction [*Chalmers et al.*, 1981; *Geerts and Raes*, 2009]. Rainfed agriculture is included in the framework as an extreme case, where any level of water stress is allowed to occur without intervention. Depending on the technology used for water distribution, each irrigation application may either provide a set amount of water, thus restoring an adequate plant or soil water level (furrows or sprinkled systems, i.e., "traditional irrigation") or supply enough water to balance current losses through evapotranspiration until the next rainfall event occurs (drip/trickle, bubbler, or microspray systems), i.e., modern microirrigation [*Vico and Porporato*, 2010]. To a first approximation, these irrigation strategies can be described by means of two parameters: a soil moisture threshold which triggers the irrigation application ("intervention point," $\tilde{s}$), and the amount of water applied at each treatment or, equivalently, the soil moisture level restored by the irrigation application target level, $\hat{s}$) [*Vico and Porporato*, 2011a]. This description also includes rainfed agriculture as the extreme case when the intervention point decreases to zero.

With these premises, the soil moisture probability density function for a generic irrigation scheme can be obtained by noting that the frequency of upcrossing and downcrossing of a generic soil moisture threshold must be equal at steady state [*Vico and Porporato*, 2011a]. This stochastic soil moisture description of irrigation provides the average irrigation requirements for a given soil, crop, and type of climate and the related water balance. This framework can be readily coupled to a minimalist model of yield and an economic balance, allowing the assessment of a variety of irrigation strategies in terms of water conservation, crop productivity, and profitability, under current and future rainfall patterns [*Vico and Porporato*, 2011b]. Specifically, the average crop yield is described as a sigmoidal function of cumulated seasonal transpiration [*Vico and Porporato*, 2015].

Figure 5a shows the role of rainfall patterns on required irrigation volumes, yields, and net economic gains for deficit traditional irrigation (black lines) and deficit microirrigation (gray lines). As a specific example, we consider corn, a drought-sensitive food staple and source of biofuels. In Figure 5a, average rainfall frequency, λ, is varied while average rainfall depth, α, is kept constant. Hence, total rainfall over the growing season increases on the abscissa of Figure 5a as rainfall frequency increases. A decrease in rainfall frequency (and rainfall totals) results in an increase in irrigation water requirements (dashed lines) and a decrease in yields and economic profits (dotted and solid lines) for both traditional and microirrigation. Nevertheless, the deficit microirrigation tends to result in lower average water requirements, but also lower yields and net economic gains than the deficit traditional irrigation. The lower yields are the result of soil moisture being maintained at the intervention point during the irrigation applications, without the beneficial excursion to higher values of soil moisture typical of traditional irrigation. For the same reason, microirrigation yields are more sensitive to changes in rainfall frequency than traditional irrigation. The lower yields of microirrigation, combined with its higher installation and maintenance costs, results in lower profits than traditional irrigation. In fact, the water savings typical of microirrigation are not sufficient to offset the higher investment costs associated with this irrigation method [*Vico and Porporato*, 2011a].

This pattern may change should the water costs increase beyond current levels, as explored in Figure 5b, which reports the amount of water per irrigation treatment that maximizes net economic return for stress-avoidance irrigation as a function of rainfall frequency across a gradient of water costs. Larger application depths are obtained by surface irrigation, intermediate depths with sprinkler systems, while the more sophisticated microirrigation is necessary for very shallow water applications. When looking at a continuum from microirrigation (small application depths, high investment costs, low water use) to traditional irrigation (large depths, lower investment costs, large water use), we can define an optimum practice based on economic metrics. Nevertheless, for current crop prices and in the absence of subsidies, negative returns (shaded area in Figure 5b) may occur for medium-to-high water costs, in particular at the lower rainfall frequencies, when variable irrigation costs associated with water applications become extremely relevant. These economic results have significant implications under projected climate changes, as a decrease in rainfall frequency may render microirrigation the most economically viable strategy.

The challenge is now to extend these methods to assess alterations of ecosystem services by irrigated agriculture. For example, *Vico and Porporato* [2010, 2011b] quantify increases in percolation due to irrigation under random rainfall, but did not address the consequences for biogeochemistry (including carbon sequestrations and soil biodiversity), leaching of nutrients, potential for soil salinization, and downstream impacts on groundwater, streams, and wetlands. A first step in this direction is to couple these dynamics to those of soil water solutes, as described next.

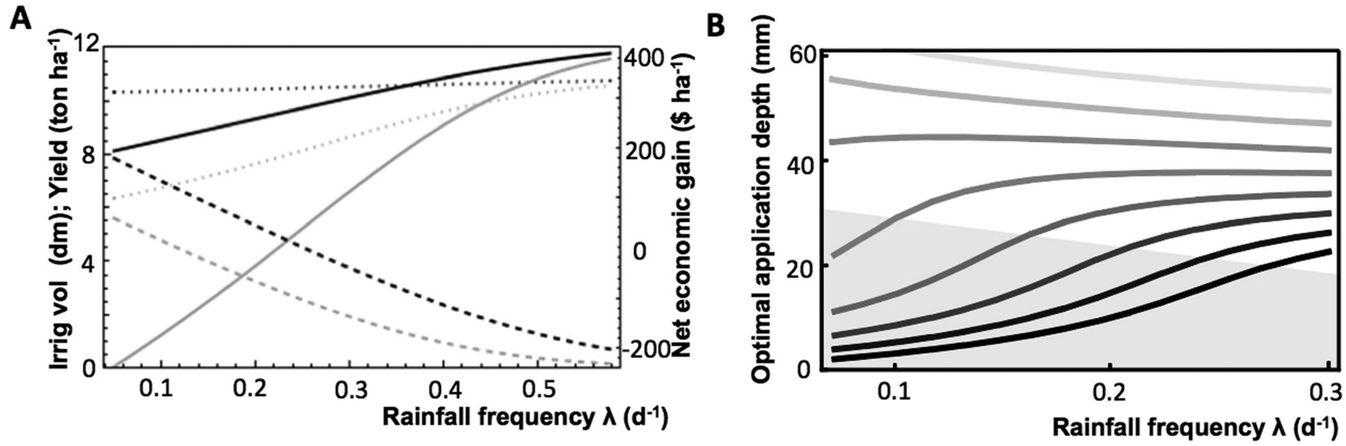

Figure 5. Impact of rainfall frequency (and rainfall total) on (a) average required irrigation volumes (dashed lines), yields (dotted lines), and economic profits (solid lines) for deficit traditional irrigation (black lines; $\tilde{s}=0.2$, $\hat{s}=0.62$) and deficit microirrigation (gray lines; $\tilde{s}=0.2$, $\tilde{s}=\hat{s}$) and (b) the most economically beneficial strategy as a function of water cost, increasing from top to bottom (ranging from 200 \$ m^{-1} ha^{-1} for light gray line to 1000 \$ m^{-1} ha^{-1} for black line). Average rainfall depth is set at $\alpha=15$ mm; evapotranspiration losses are modeled with a piecewise linear function [*Rodriguez-Iturbe et al.*, 1999]. The parameters of application efficiency, crop yield, and economic models are listed in Table 1 of *Vico and Porporato* [2011b]. In Figure 5a, the cost of water is set to 148 \$ m^{-1} ha^{-1}, corresponding to the average U.S. expense for irrigation water from off-farm suppliers in 2003 [*USDA-NASS*, 2003, Table 22]. In Figure 5b, shaded area refers to parameter combinations for which the economic return is negative.

3.2. Soil Water Quality: From Fluctuations Under External Forcing to Macroscopic Equations

The external stochastic forcing through rainfall and the nonlinear coupling between soil moisture and solute concentration make the behavior of the stochastic system of equations (4) and (5) difficult to predict theoretically, despite the limited number of parameters. While numerical solutions of the two-equation system may already yield practical insights, theoretical analysis would be especially useful to investigate general behaviors and understand the role of climatic drivers and internal dynamics. For example, when there is a clear separation of time scales between soil moisture temporal evolution and the duration of leaching events, it is possible to treat the two equations separately by first solving the stochastic differential equation of soil moisture and then approximating the short-duration leaching events as independent, instantaneous events whose frequency is controlled by the probability of reaching percolation thresholds [*Manzoni et al.*, 2011; *Suweis et al.*, 2010].

Alternatively, one can resort to a so-called "macroscopic approach" and take the ensemble average of each term in equations (4) and (5):

$$\begin{aligned} nZ_r\frac{d\langle s\rangle}{dt} &= \langle R\rangle+\langle I\rangle-\langle T\rangle-\langle L\rangle \\ \frac{d\langle m\rangle}{dt} &= \langle I_m\rangle+\langle I_a\rangle+\langle \phi\rangle-\langle U\rangle-\langle P\rangle-\langle V\rangle. \end{aligned} \tag{6}$$

This approach is typical in complex systems and has been extensively used in statistical mechanics [e.g., *Van Kampen*, 1992] and turbulence modeling [e.g., *Pope*, 2000]. Analyzing this system requires overcoming a "closure problem," wherein the flux terms cannot be expressed in terms of the means $\langle s\rangle$ and $\langle m\rangle$ because of nonlinearities, but involve higher-order, joint moments of s and m. Thus, to evaluate equations (6), simplifying assumptions are needed on the functional forms of these ensemble fluxes, as was discussed by *Laio et al.* [2002] and *Feng et al.* [2015] for the case of seasonal changes in the ensemble soil moisture. The potential advantages provided by overcoming the closure problem would be remarkable in that the resulting equations are deterministic dynamical systems that naturally embed the effect of stochastic external forcing while being amenable to dynamical system analysis. It is however very difficult to find parameterization of mean fluxes in (6) that are suitable for a wide range of climate, vegetation, and soil conditions. A few preliminary examples, intended to be a "proof of concept" of this approach, are presented in the following subsections.

3.2.1. Soil Salinization

When m represents soluble minerals, the coupled system of equations (4) and (5) may be used to analyze probabilistically the long-term dynamics of soil salinization. First, we consider primary salinization caused by accumulation of naturally occurring salts. Secondary salinization is then considered by adding anthropogenic salt inputs via irrigation.

For primary salinization, the macroscopic equations (6) are rewritten without irrigation and solved at steady state as:

$$\begin{gathered}\langle R(t)\rangle=\langle T(t,s(t))\rangle+\langle L(t,s(t))\rangle\\ \langle I_m(t)\rangle=K_d\kappa\langle C(t)\cdot T(t,s(t))+K_dC(t)\cdot L(t,s(t))\rangle\end{gathered}. \tag{7}$$

Here K_d is the partition coefficient between adsorbed and dissolved fractions, κ the transpiration stream concentration factor or the ratio of the concentration in the transpiration stream to that in soil water [*Dietz and Schnoor*, 2001], and $C=m/(nZ_rs)$ is the concentration of dissolved salts in the soil. We approximate plant uptake to be linearly dependent on soil moisture over large spatial areas, where *PET* is the potential evapotranspiration, thus $\langle T\rangle=PET\langle s\rangle$. We also approximate the leakage rate using a modified first term of its Taylor expansion [*Feng et al*., 2015; *Laio et al*., 2002] such that $\langle L\rangle=\frac{\lambda}{\gamma}\ e^{-\gamma\varepsilon(1-\langle s\rangle)}$, where γ is a normalized soil rooting depth defined by $\gamma=nZ_r/\alpha$ and ε accounts for the bulk effects of other soil features. Furthermore, for illustration we assume negligible cross covariance between salt concentration and soil water fluxes, such that $\langle C\cdot L\rangle\approx\beta\langle C\rangle\langle L\rangle$ and $\langle C\cdot T\rangle\approx\beta\langle C\rangle\langle T\rangle$, where β serves as a linear correction factor. The effect of the climate is summarized by the nondimensional dryness index, defined as the ratio of long-term potential evapotranspiration to rainfall, i.e., $D=PET/\langle R\rangle$. Then, the steady state ensemble average concentration of salt under these conditions can be found as a function of the dryness index,

$$\langle C\rangle=\frac{\langle I_n\rangle}{K_dPET\ \ \beta\ \left(\kappa\langle s\rangle+De^{-\gamma\varepsilon(1-\langle s\rangle)}\right)}. \tag{8}$$

The results are shown in right plot of Figure 6, where the steady state salt concentration $\langle C\rangle$ is plotted against increasing dryness index D for different values of the potential evapotranspiration. The increase in D comes as a result of decreasing mean rainfall frequency, λ, while mean rainfall depth, α, is kept constant. Primary salinization is especially pronounced in drier climates (high D) where potential evapotranspiration greatly exceeds rainfall that may leach salt out of the soil. Indeed this trend is even more accentuated in locations with lower potential evapotranspiration where, at the same D, rainfall rates are comparatively even lower (as seen in some higher latitudes in the left plot of Figure 6).

Conditions leading to the accumulation of salts in soils due to irrigation (secondary salinization) have been determined by ad hoc field experiments and numerical simulations [*Ayars et al*., 1993; *Bresler et al*., 1983; *Corwin et al*., 2007; *Schoups et al*., 2005; *Straw et al*., 2005]. Related economic considerations and exploration of optimal allocation strategies to reduce risk of secondary salinization have also been presented in the literature [*Bras and Cordova*, 1981; *Matanga and Marino*, 1979; *Yaron et al*., 1980]. Several spatially (vertically and/or horizontally) explicit numerical models have also been developed [*Corwin et al*., 2007; *Schoups et al*., 2005; *Straw et al*., 2005], simulating unsaturated soil water flow via Richards' and solute transport equations. Such models however require precise site-specific parameterizations and are computationally demanding, especially when the goal is to analyze the likelihood of salt buildup under future climate.

To consider the role of irrigation, it is instructive to compare the results provided by the crude macroscopic approximation that neglects the effects of cross correlations between the fluctuations of soil moisture and salt (i.e., only the feedback between averages is retained) to those from numerical analysis of the full coupled dynamics of irrigation and soil salinization under stochastic rainfall described by equations (4) and (5). Intuitively, irrigation can be thought of as playing two contrasting roles in regulating soil salt concentration. On the one hand, irrigation introduces an additional source of salt through those dissolved in the irrigation water (the term I_a in equation (6) now designates the concentration of salt in the irrigation water). On the other hand, irrigation increases soil moisture, which leads to an increase in leaching and salt flushing from the soil that may overcome the effects of increased salt input into the soil. Using similar approximations as those adopted in equation (8) for primary salinization, the macroscopic equation describing salt concentration under secondary salinization, under negligible primary salt input, can be easily computed as:

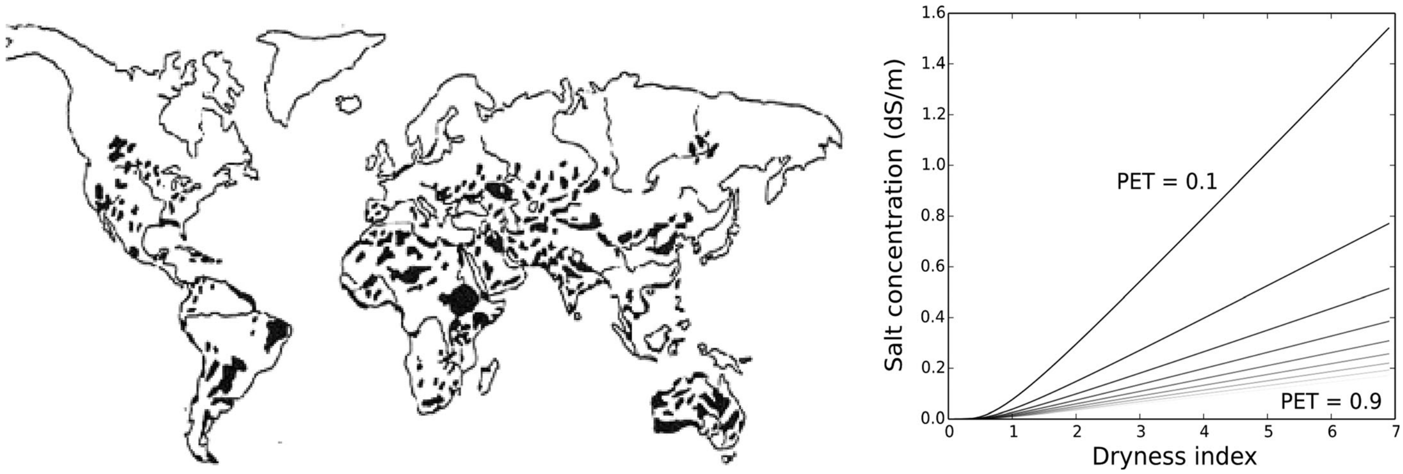

Figure 6. (left) Global distribution of salt affected soils (adapted from *Szabolcs* [1989]). (right) The steady state concentration of salt as defined in equation (8) plotted against the climatic dryness index D (or the ratio of potential evapotranspiration to rainfall). Each line corresponds to changes in the potential evapotranspiration (in mm/d) varying from low (dark lines) to high (light lines), while mean rainfall depth is kept constant at $\alpha=10$ mm/d.

$$\langle C\rangle=\frac{C_l n Z_r\langle I\rangle}{K_d PET\ \ \beta\left(\kappa\langle s\rangle+De^{-\gamma\varepsilon(1-\langle s\rangle)}\right)}, \tag{9}$$

where the connection between anthropogenic input of salt, $\langle I_a\rangle$, through irrigation $\langle I\rangle$ is established by setting $\langle I_a\rangle=C_l n Z_r\langle I\rangle$, with C_l as the salt concentration in the irrigation water.

The results for the salt concentration in the soil $\langle C\rangle$ described by equation (9) are shown in Figure 7a as a function of the average irrigation rate I for different values of the dryness index D. As can be seen in Figure 7a, the concentration of salt in the soil is determined by both the climate and the irrigation rate. Particularly under drier climates, a maximum for the soil salt concentration exists at an intermediate rate of irrigation, due to the opposing effects of irrigation and leaching. In drier climates, salt in the irrigation water increases the soil salt concentration. As irrigation is increased, however, enhanced leaching counterbalances the additional salt input, and soon the salt concentration decreases again. In contrast, in wetter climates, leaching events due to naturally occurring rainfall already dominate the system such that the overall salt mass balance is not as drastically affected by the increase through irrigation. As such, the maximum observed in drier climates ceases to appear. A comparison of the approximate analytical solutions and the numerical simulation of the complete system, in which the covariance of salt mass and soil water fluxes (e.g., $\langle C\cdot L\rangle$ and $\langle C\cdot T\rangle$) are explicitly taken into account, reveals that the behavior of the system and the existence of the maximum concentration are consistent across different climate regimes (Figures 7b and 7c).

Extensions of the previous analysis could include plant feedbacks on soil salinity. In some salt tolerant species (e.g., dates and some vegetables), a moderate increase in salinity may actually promote growth, which nevertheless decreases at extreme salt levels. However, in most species salinity at least triggers stomatal closure and reduced growth [*Munns and Tester*, 2008; *Volpe et al.*, 2011]. Therefore, reduced transpiration in saline conditions may affect the long-term soil moisture balance. Analysis of long-term salinization trends can also inform current efforts toward salt tolerant plants and accounting for future climate scenarios will be key to assess sustainability of agricultural practices at large scales, including groundwater dynamics [*Hillel*, 1998; *Jobbágy and Jackson*, 2001].

3.2.2. Managing Soil Mineral Dynamics: Fertilization and Phytoremediation

After irrigation, soil fertilization by addition of mineral nutrients and N-rich organic amendments is the second main form of acceleration of soil-plant dynamics (Figure 1). While it played a pivotal role in the so-called green revolution, making it possible to dramatically increase food production, such unprecedented inputs of nitrogen, phosphorous, and potassium to agricultural soils have also altered the natural biogeochemical cycles, resulting in diffuse eutrophication [*Vitousek et al.*, 1997] and contributing to greenhouse gas accumulation. Once in the ecosystems (either natural or managed), the concentrations and fate of nutrients depend on climate and its interactions with vegetation and soil biota. Not only

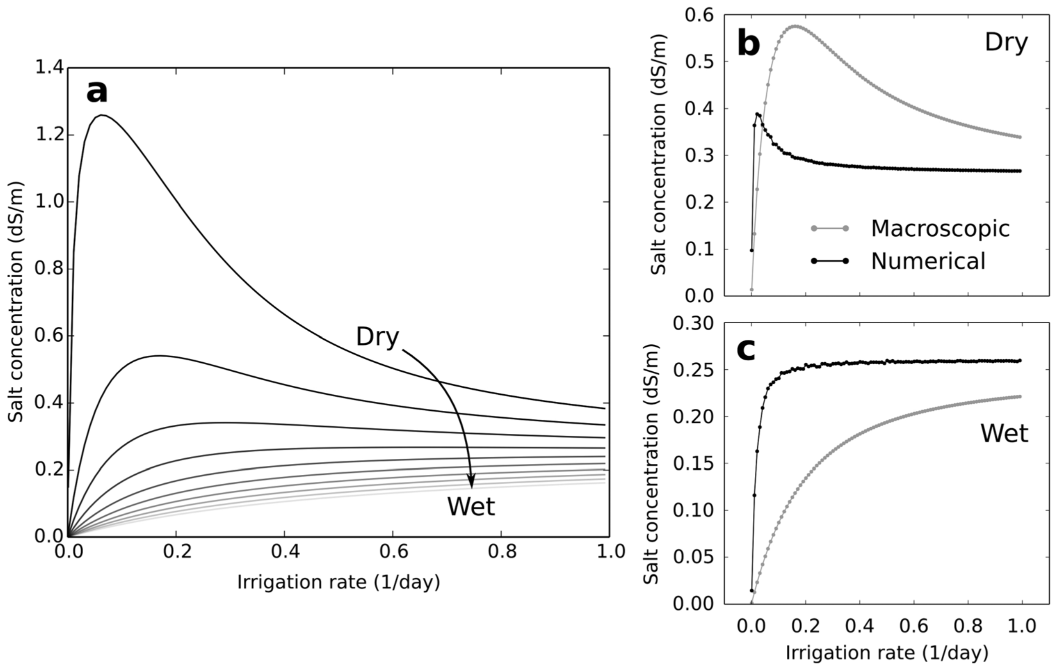

Figure 7. (a) Mean salt concentration as a function of irrigation rate for different climate conditions (using the macroscopic equation (9)), where "Drier" and "Wetter" conditions span the range, respectively, from $D=50$ to $D=0.55$. (b and c) Comparison of the salt concentration-irrigation rate relations obtained from the macroscopic solution of equation (9) (gray lines) and its corresponding numerical solution in which the covariance of salt mass and soil water fluxes are explicitly simulated (black lines). The dryness index is $D=5$ in Figure 7b and $D=1$ in Figure 7c. Other parameters: $c_I=1000$ mg cm^{-1} m^{-2}, $n\ Z_r=15$ cm, $PET=0.5$ cm/d, $\alpha=1.0$ cm, $\kappa=0.1$, and $K_d=0.6$, $\varepsilon=0.1$, $\beta=16$.

does soil moisture play a major role in controlling the balance of nutrient uptake by vegetation and leaching (similarly to the balance of soil contaminants described below), it also impacts mineral N production through mineralization of soil organic matter [*Austin et al.*, 2004; *Linn and Doran*, 1984].

The amount of fertilizer that needs to be supplied to maximize profit is strongly linked to hydrologic variability [*Paulson and Babcock*, 2010]. While data-driven, plot and watershed-scale models to predict soil N fate are common in the literature [e.g., *Birkinshaw and Ewen*, 2000; *Maggi et al.*, 2008], stochastic approaches are fewer [*Botter et al.*, 2008; *Manzoni and Porporato*, 2009, and references therein; *Porporato et al.*, 2003]. These studies deal with the stochastic analysis of equations (4) and (5), or extended versions thereof, in which the solute m is taken as the amount of soil nitrates. In contrast, agricultural economic models at the yearly time scale often account for exogenous (e.g., spatial or climatic) variability, but tend to neglect its mechanistic basis (e.g., how rainfall stochasticity propagates through the ecosystem compartments). Others studied optimal fertilization strategies in the presence of environmental variability that affects crop yield both directly and indirectly through human decisions [*Lehmann et al.*, 2013; *Paulson and Babcock*, 2010] as well as modification of plant ecophysiological traits governing N uptake and use efficiencies, which can be potentially applied toward more sustainable agriculture [*Weih et al.*, 2014; *Xu et al.*, 2012].

Plants have also been used to stabilize, extract, degrade, or promote the volatilization of soil contaminants [*Dietz and Schnoor*, 2001; *Gerhardt et al.*, 2009; *Pilon-Smits*, 2005; *Salt et al.*, 1998]. Phytoremediation refers to the use of plants to remove contaminants from soils through the U term in equation (5). Phytoremediation, however, has two major downsides, (i) longer durations than traditional techniques, and (ii) potentially high contaminant leaching losses. To quantify the long-term mean extraction duration, $\langle\tau\rangle$, and efficiency, $\langle\chi\rangle$ (amount of contaminant extracted by plants over total contaminant loss), equations (4) and (5) have been solved under stochastic rainfall, showing that $\langle\tau\rangle \sim \langle\chi\rangle/\langle T\rangle$ [*Manzoni et al.*, 2011]. The extraction process may be lengthy because plants are intrinsically slow in taking up contaminants and might suffer from other environmental stresses as well (e.g., droughts) [*Gerhardt et al.*, 2009]; as a consequence, larger transpiration rates associated with favorable conditions accelerates the phytoremediation process (the denominator in the above equation for $\langle\tau\rangle$). Moreover, for a given rainfall rate, higher transpiration implies lower percolation and thus lower leaching losses. In turn, lower leaching increases phytoremediation efficiency, which lengthens the extraction duration (captured by the numerator $\langle \chi \rangle$). Therefore, a tradeoff emerges between speed and efficiency, such that fast remediation is possible only with substantial leaching, which might affect downstream water bodies [*Koopmans et al*., 2007; *Pilon-Smits*, 2005]. Along gradients of increasing rainfall, leaching losses increase more than linearly, resulting in lowered remediation efficiency, a pattern consistent with short-term experiments [*Grčman et al*., 2001]. Hence, also along climatic gradients a tradeoff emerges between remediation duration and efficiency that has rarely been investigated.

4. Sustainable Use of Soil and Water Resources as a Problem of Optimal Stochastic Control

Any effort to sustainably manage water and soil resources requires finding optimal solutions under multiple constraints in systems that are forced by unpredictable climatic, biological, and social dynamics. Toward this goal, the methods of optimal stochastic control (or robust control) and probabilistic risk analysis may prove to be valuable. In turn, the complexity of the ecosystem-society interaction (section 2) may pose novel challenges for exciting theoretical developments in these fields, which have been traditionally confined to more clearly defined engineering and industrial problems.

In general, optimal control theory aims at finding a strategy that minimizes (respectively, maximizes) a given cost (gain) functional, based on generalizations of the calculus of variations by Pontryagin and Bellman among others [*Pesch et al*., 2009; *Sussmann and Willems*, 1997]. Optimal control applications abound in science, engineering, and industry, including fishery management, pollution control, capital accumulation problems, and oil drilling [*Sethi and Thompson*, 2006]. However, only a few examples of control theory applications in the context of environmental problems can be cited [e.g., *Lehmann et al*., 2013; *Mannocchi and Mecarelli*, 1994; *English*, 1990]. Ecological theories also employ optimization approaches to explain plant and microbial functioning, on the grounds that natural selection favors organisms that optimize use and allocation of limiting resources [e.g., *Cowan*, 1986; *Eagleson*, 2002; *Manzoni et al*., 2013, and references therein; Rodriguez-Iturbe and Porporato, 2004]. In what follows, we expand on one specific example for illustration.

4.1. The Example of Saline and Sodic Soil Remediation

The problem of remediation of saline and sodic soils offers an interesting example where optimal control can be applied neatly with the quality of the irrigation water as the control parameter. The use of brackish or slightly saline water is common in arid and semiarid regions [*Assouline et al*., 2015], and an optimal management of soil salinity and sodicity can involve changing the irrigation water properties in time, e.g., by mixing costly freshwater to the available brackish water, or by dissolving amendments like gypsum in the applied irrigation water. Here as an example, we consider the case of irrigation water quality altered by adding calcium cations using soil amendments such as gypsum. More specifically, we consider the remediation of a sodic soil (Exchangeable Sodium Percentage, ESP $>$ 15%, and specific electrical conductance, $K < 4dS/m$), seeking the optimal calcium amendment strategy that remediates the soil in the least possible time by exchanging sodium ions with calcium ions. We first develop dynamical equations for the soil salinity and sodicity of an irrigated plot, based on the macroscopic approach by *Mau and Porporato* [2015] and then address the optimal control problem. We only summarize the main results here, and defer the details of the theory and its implementation to a later contribution.

Assuming that under stress-avoidance microirrigation, soil moisture remains relatively constant at $\bar{s}$, the soil moisture balance of equation (4) becomes simply $L=I-T$, where $L(s)=K_s s^c$ is the percolation rate, K_s is the saturated hydraulic conductivity, and the exponent c depends on soil properties. The dynamics of salinity and sodicity can be found by considering the total salt balance and sodium balance, respectively. Salt is assumed to enter the root zone exclusively through irrigation and leave the system only through leaching to deeper soil layers. Accordingly, the balance equation (5) for salt in solution simplifies to:

$$\frac{dq_s}{dt}=I_a-(I-T)C, \tag{10}$$

where q_s is the total amount of salt cations per unit area (expressed as molar charge), $C=q_s/(nZ_r\bar{s})$ is the salt concentration, and $I_a=I\ C_I$ is the rate of salt addition via irrigation (with C_I indicating the salt concentration of irrigation water). Note that because we distinguish between different cations (Ca and Na), it is more convenient to use molar charge rather than mass. The relation $m^X = q^X M^X / v^X$ transforms molar charges q^X into grams of mass m^X of cation X, where M is the molar mass and v is the valence. Equation (10) can be rewritten to describe the evolution of salt concentration C,

$$\frac{dC}{dt} = \frac{1}{n\ Z_r\ \bar{s}}[I\ C_I - C(I-T)], \tag{11}$$

The linear differential equation above governs the behavior of soil salinity, and is dependent upon the control parameter C_I.

The dynamics of soil water sodicity is influenced by its coupling to the exchange complex that can act as a buffer of sodium cations. For illustration, we describe only sodium and calcium. Sodium and calcium cations adsorbed to soil particles of the exchange complex—respectively, q_x^{Na} and q_x^{Ca}—can be replaced by sodium and calcium in the soil solution—respectively, q_s^{Na} and q_s^{Ca}. The exchange reaction of cations between soil solution and exchange complex is much faster than the typical time scale of sodification, therefore the cations of both phases are considered to be in thermodynamic equilibrium given by the Gapon equation (see details in *Mau and Porporato* [2015]). With appropriate substitutions and mathematical developments [*Mau and Porporato*, 2015], the dynamical equation for ESP, denoted E, is:

$$\frac{dE}{dt} = \frac{I\ C_I E_I - (I-T)Cg_s - n\ Z_r \bar{s} \frac{dC}{dt}\left[g_s + C\frac{\partial g_s}{\partial C}\right]}{C_{EC}\ M + n\ Z_r \bar{s} C \frac{\partial g_s}{\partial E}}, \tag{12}$$

where $\frac{dC}{dt}$ is given in equation (11), C_{EC} is the cation-exchange capacity, M is the mass of dry soil per unit area, and the function g_s reads

$$g_s = \frac{2}{1 + \sqrt{1 + 8K_g^2 C(E^{-1}-1)^2}}. \tag{13}$$

Equation (12) is nonlinear in the variables E and C, and also depends nonlinearly upon the irrigation parameters C_I and E_I (the equivalent fraction of sodium in irrigation water). Equations (11) and (12) form a two-dimensional nonlinear system, which can be rewritten in a more compact form as

$$\begin{aligned} \frac{dE}{dt} &= h_1(E, C; C_I, E_I) \\ \frac{dC}{dt} &= h_2(C; C_I) \end{aligned} \tag{14}$$

representing the temporal evolution of salinity C and sodicity E.

With equations (14), the problem of optimal control can now be addressed. By dynamically changing the quality of irrigation water, i.e., varying the value of E_I and C_I, we wish to rehabilitate a sodic soil (i.e., to salinity and sodicity levels within a range suitable for plant growth, $C < 40$ meq/L and $E < 0.15$) in a minimal amount of time. For an addition of calcium cations J_g (meq of calcium cations per day per unit area), the salinity and sodicity of irrigation water vary according to:

$$\begin{aligned} E_I &= \frac{E_I^0}{1 + \frac{J_g}{C_I^0 I}}, \\ C_I &= C_I^0 \frac{J_g}{I}, \end{aligned} \tag{15}$$

where E_I^0 and C_I^0 denote the sodicity and salinity of irrigation water when no calcium additive is introduced, respectively. Thus, substituting equations (15) into equations (14), a system of equations that depends on a single control parameter, namely J_g, is obtained.

The optimal control problem finds an amendment strategy $J_g(t)$ that takes the system from a sodic soil $x_1 = (E_1, C_1)$ to a remediated soil $x_2 = (E_2, C_2)$ in the minimal amount of time, given that the calcium supplement stays in the range $0 < J_g(t) < J_g^{max}$, where J_g^{max} is the maximal rate of calcium cations added to irrigation

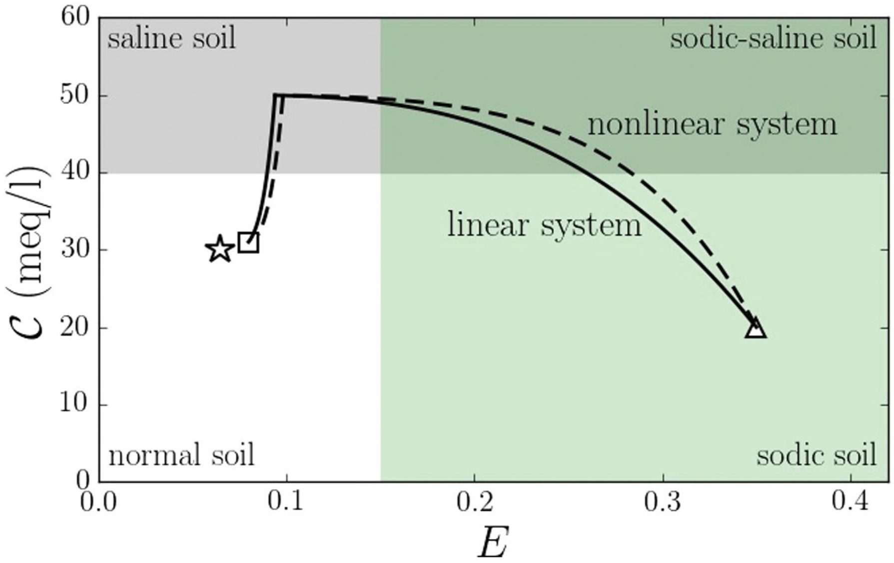

Figure 8. Optimal trajectory in the salinity-sodicity phase space (E, C) for remediating a sodic soil in minimal time. The initial condition is marked with a triangle, the goal state with a square, and the steady state of equation (16) with a star. The solid trajectory denotes the analytical optimal solution of (14), and the dashed trajectory is a simulation of the nonlinear system of equations (14), for the same calculated switching strategy. Parameters: $n=0.43$, $Z_r=300$ mm, PET = 5 mm/d, M = 450 kg/m^2, $C_{EC}=100$ meq/kg, $K_g=0.01475$, I = 10 mm/d, $E_I^0=0.45$, $C_I^0=15$ meq/L, and $J_g^{max}=100$ meq/m^2/d.

water. In order to proceed analytically, we first substitute the parameters E_I and C_I by equations (18), then linearize the system around its stable point, and finally linearize the dependence of the system on the control parameter J_g around the point $J_g^0=0$.

The resulting system of equations reads:

$$\frac{dx}{dt}=f(x)+G(x)J_g, \tag{16}$$

where $x=(E, C)$ and for all physical values of the parameters of the problem, the vectors $f(x)$ and $G(x)$ yield:

$$\begin{aligned} f(x)&=\left(f_E^0+f_E^1 E, f_C^0+f_C^1 C\right), \\ G(x)&=\left(G_E^0+G_E^1 E, G_C^0\right), \end{aligned} \tag{17}$$

which effectively decouples the sodicity equation from the salinity equation. Equations (16) and (17) represent a *normal* linear control system, which means that the control $J_g(t)$ has a so-called bang-bang solution, i.e., its values are restricted to the extremes of the range $0 < J_g(t) < J_g^{max}$, with abrupt transitions between them [*Liberzon*, 2011; *Stengel*, 2012]. It can be shown that, as long as the initial sodicity is greater than the steady state sodicity prescribed by equation (16), the switch of the optimized control parameter occurs once, from an "on" state ($J_g=J_g^{max}$) to an "off" state ($J_g=0$) at the switching time t_s.

Figure 8 shows the temporal evolution of C and E for the optimal remediation strategy, in the salinity-sodicity phase space, starting from $E=0.35, C=20$ meq/L (denoted by a triangle) with a final target state $E=0.08, C=31$ meq/L (denoted by a square). For the parameter values chosen, the switching time is on day 109, and the remediation duration is 161 days. The trajectory starts from sodic conditions, transitions to sodic-saline conditions as sodium is substituted by calcium, and eventually reaches saline conditions when Na concentrations decrease below 0.15 meq/L. Finally, as calcium amendments are stopped at t_s (while irrigation with clean water continues), the soil switches to the desired normal condition suitable for cultivation. The solid line is obtained via the linearized system, while the dashed trajectory is a simulation of the original nonlinear system of equations (14) with the same switching strategy calculated for the linearized equation (16). The comparison in Figure 8 shows that, although simplified, the trajectory of the linearized system (16) is able to capture the dynamics of the nonlinear system reasonably well. This means that the optimal control analysis shown here can be useful in guiding restoration efforts of sodic soils.

5. Conclusions

The previous examples demonstrate the interplay of stochastic components, thresholds, and nonlinearities in the coupled dynamics of water, vegetation, and nutrients or contaminants in soils, which are typical of ecohydrological processes in both natural and managed ecosystems. We have advocated for a parsimonious approach to their modeling, in which suitable simplifications may allow one to perform theoretical analyses displaying the governing groups of soil, climate, and crop parameters and show how water and nutrient cycle management may alter the relative importance of various fluxes (section 3). The use of macroscopic equations for the moments of stochastic ecohydrological variables seems particularly promising for its balance of complexity and parsimony. This approach, often adopted in the study of stochastic processes [e.g., *Gardiner*, 1986; *Van Kampen*, 1992], is similar to the use of Reynolds-averaged Navier-Stokes equations in turbulence modeling [*Pope*, 2000]. In our examples here, the "closure problem" resulting from the nonlinear coupling of stochastic variables has been solved quite simplistically, by neglecting the covariance of soil moisture and nutrient or contaminant solute. Much theoretical research is needed to clarify the role of these covariances and to develop systematic closure methods for ecohydrological moment equations, especially when additional equations with soil organic matter and microbial dynamics are involved [Porporato et al., 2003]. Along these lines, and more generally, the application of model reduction techniques to the often too complex environmental models will help develop low-dimensional models integrating fast and slow time scale dynamics for the most relevant variables (see, e.g., the recent developments in applied mathematics and physics in *Crommelin and Majda* [2004], *Givon et al*. [2004], *Schmuck et al*. [2013], and *Tartakovsky et al*. [2011]), with potentially important improvements in calibration, numerical capabilities, and analytical developments.

The mathematical analysis of ecosystem and human interaction exemplified in section 2 is still in its infancy, but may have great potential to improve understanding of the long-term consequences of altering human pressure on the environment and water resources, especially when coupled to more detailed "agent-based models" of human behavior [e.g., An, 2012]. We also tried to frame the problem of soil and water resources management using the theory of optimal stochastic control (section 4). Here the challenge of including multiple objectives or constraints dealing with sustainability and profitability that necessarily involve human factors is again compounded by the fact that these problems often involve uncertainties in the system's parameters and forcings, thus requiring so-called robust control techniques to make the cost functionals relatively insensitive to fluctuations [*Anderies et al*., 2007; *Rodriguez et al*., 2011]. Along these lines, the methods of uncertainty quantification [*Tartakovsky*, 2013] may add relevant avenues of both theoretical and applied research.

Several additional problems and process interactions were not mentioned in this article: for example, the problem of plant trait optimization given climate and soil conditions and related projected changes; the optimization of irrigation within the broader scope of soil biogeochemistry, as it relates to carbon storage, nutrient retention, productivity, and salinization; and finally, the optimal management of spatial heterogeneity to minimize the effects of habitat fragmentation on biodiversity and ecosystem services. In all of these problems—similarly to the examples discussed in this paper—the different disciplines brought together by ecohydrology, complemented by methods of environmental engineering, stochastic processes, nonequilibrium statistical mechanics, and control theory, may help provide a scientific foundation to develop policies and strategies toward sustainable ecosystem management.

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