Exploratory system dynamics: a directed search for limits to global water use

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Abstract: Rockström et al. (2009) introduced the concept of a safe operating space for humanity that will not push the planet out of the 'Holocene state'. These limits are being investigated for various earth bound systems. Estimates of these limits are plagued by uncertainty. In case of the limits to the world water system, these uncertainties arise out of conflicting models, regional variations, limitation of expansion of water use through financial and institutional capacity, uncertainty about the realization and efficiency of trans-boundary water transfers, and interdependency between the water system and other earth systems. This paper aims at investigating the limits to global freshwater use. To this end, the behavior of a System Dynamic model of the world water balance is explored across a wide variety of uncertainties. Active non-linear testing is used to identify the best case and worst case for water stress and world population. We find counter intuitive results related to the occurrence of maximum water stress, conclude that global limits can be investigated with a spatially aggregated model and are strengthened in our hypotheses that exploratory modeling adds to the understanding of complex and uncertain issues in a way that predictive approaches cannot.

Keywords: ANEMI, system dynamics, exploratory modeling and analysis, world water models, safe operating spaces, Holocene state

1 Introduction

In the *Nature* article 'A safe operating space for humanity', Rockström et al. (2009) introduce the concept of a safe operating space for humanity. A safe operating space is the space for human activities that will not push the planet out of the 'Holocene state' that has seen human civilizations arise, develop, and thrive. The concept is inherently anthropocentric and excludes non-human events and processes that could push the planet out of the Holocene state. Rockström et al. have identified nine earth-system processes and associated thresholds which, if crossed, are expected to generate unacceptable environmental change. These include climate change, rate of biodiversity loss, interference with the nitrogen and phosphorus cycles, stratospheric ozone depletion, ocean acidification, global freshwater use, change in land use, chemical pollution, and atmospheric aerosol loading. For all nine earth-system processes identified associated preliminary boundaries are given by Rockström et al. (2009). However, for only three of them, notably, climate change, rate of biodiversity loss, and the nitrogen cycle, these boundaries are substantiated theoretically and methodologically. The thresholds for the other six, including the global fresh water cycle, are tentative 'best guesses'

(Rockström et al. 2009). For water, Rockström et al maintain that the boundary must be set to safely sustain enough green water for moisture feedback while allowing for terrestrial and aquatic ecosystem functioning and as a first attempt propose runoff depletion in the form of consumptive blue water use as a proxy. Based on global fresh water cycle assessment studies, Rockström et al set the threshold for global fresh water use at a range of 4000 to 6000 cubic kilometers per year. The current (2009) global fresh water use is estimated at 2600 cubic kilometers per year (Rockström et al. 2009).

Although we do subscribe to Rockström et al.'s ambition and concepts, there are nevertheless several problems associated with the approach they advance. A first problem is the ambiguous treatment of reductionism . While the authors clearly recognize thresholds and threshold behavior as a systemic and emergent property, Rockström at al. embark on a reductionist approach by reducing the earth system to nine biophysical processes and define planetary boundaries internal to these subsystems. Such an approach is bound to overlook the impacts of the dynamic interactions between the subsystems. To this, Molden (2009) adds that the concept of a global limit overlooks the importance of local conditions, regional variations, the role of management, and financial and institutional capacity in magnifying or ameliorating problems. Moreover, the estimate of the global limit for blue water use is based on a limited number of studies extrapolated beyond their original intentions (Molden 2009). Furthermore, structural uncertainties exist in the relation between climate change and renewable fresh water resources (RFWR) (Oki and Kanae 2006).

From the foregoing, we conclude that the hypothesis of Rockström et al. that humanity may soon be approaching the boundaries for global freshwater use is uncertain and disputed. Most of the uncertainty is located in the data on the fresh water cycle and the scale at which they should be evaluated. Much of e the dispute relates to uncertainties in the interaction between socio-economic and physical factors in the approach used for establishing the safe operation space with respect to water use and the consequences of climate change. That is, the limits on fresh water use cannot be established without considering related subsystems and the wide variety of uncertainties. The reductionist and complex dynamics issues are tackled by utilizing an integrated System Dynamic models of the planetary fresh water cycle that takes into consideration the non-linear and dynamic feedback relationships between physical characteristics of water balance and population growth; development of agriculture and industry; technological development and use of other resources. The issue of uncertainty is addressed by applying Exploratory Modeling and Analysis (EMA), a research methodology that uses computational experiments to analyse complex and uncertain systems (Agusdinata 2008; Bankes 1993). More specifically, we perform a directed search using Active Non Linear Testing (ANT) 'to enhance the exploration of ensembles of models that incorporate a variety of plausible underlying assumptions' (Miller 1998, : 821). The remainder of this paper is structured as follow. Section 2 outlines the method in more detail. Section 3 contains the application and results. Section 4 contains an extended discussion of the results.

2 Method

2.1 Modeling the world water cycle

There are various modeling approaches that can be used to model the planetary fresh water cycle. One modeling approach that fits with the suggested holistic approach is System Dynamics (Sterman 2000; Forrester 1968). At present, several integrated System Dynamics water cycle models exist. These models have been used to define global limits to the use of blue water. AQUA (Hoekstra 1998) and WorldWater (Simonovic 2002) are the best known models. ANEMI is a more recent model in this same tradition (Davies and Simonovic 2010, 2011). These models deviate from other world water models such as WaterGap (Alcomo et al. 2003) and PCR-GLOBW (van Beek and Bierkens 2009) in that the various feedbacks between the water cycle, water use, socio economic developments, the climate, etc. are endogenous to the model. In contrast, in WaterGap for example, scenarios for population development, GDP, and electricity production are necessary inputs. This implies that models like WaterGap cannot be applied to investigate the impact of water shortages over time on how population or GDP evolves, nor can it cope with human adaptation to water shortage. For example, WaterGap will overestimate irrigation consumption in case of water shortage (Hunger and Döll 2008). This advantage of integrated dynamic world water models, however, comes at the price of not being geographically explicit.

2.2 Coping with uncertainty

The issue of uncertainty is addressed by applying EMA. EMA can be contrasted with the use of models to predict system behavior, where models are built by consolidating known facts into a single package (Hodges and Dewar 1992). When experimentally validated, this single model can be used for analysis as a surrogate for the actual system. Where applicable, this consolidative methodology is a powerful technique for understanding the behavior of complex systems. Unfortunately, for many systems of interest, the construction of a model that may be validly used as surrogate is simply not a possibility. This may be due to a variety of factors, including the infeasibility of critical experiments, impossibility of accurate measurements or observations, immaturity of theory, openness of the system to unpredictable outside perturbations, or nonlinearity of system behavior, but is fundamentally a matter of not knowing enough to make predictions (Cambell et al. 1985; Hodges and Dewar 1992). For such systems, a methodology based on consolidating all known information into a single model and using it to make best estimate predictions can be highly misleading.

EMA can be useful when relevant information exists that can be exploited by building models, but where this information is insufficient to specify a single model that accurately describes system behavior. Under these conditions, models can be constructed that are consistent with the available information, but such models are not unique. Rather than specifying a single model and treating it as a reliable image of the system of interest, the available information is consistent with a set of models, whose implications for potential decisions may be quite diverse. A single model run drawn from this potentially infinite set of plausible models is not a "prediction"; rather, it provides a computational experiment that reveals how the world would behave if the various guesses any particular model makes about the various unresolvable uncertainties were correct. By conducting many such computational experiments, one can explore the implications of the various guesses. EMA is the explicit representation of the set of plausible models, the process of exploiting the information contained in such a set through a large number of computational experiments, and the exploration and analysis of the results of these experiments. In this way, EMA aims at offering support to decision making, without falling into the pitfall of trying to predict the unpredictable.

EMA takes a particular stance on how models can be usefully applied to inform decisionmaking despite their limited predictive power. This stance is independent of the type of modeling paradigm that is being used. EMA researchers have utilized agent based models, spreadsheet models, operation research models, and domain specific modeling approaches. Recently, there has been an upsurge in combining EMA with exploratory System Dynamics models. EMA and System Dynamics are perfect partners (Pruyt 2010, 2010; Pruyt and Hamarat 2010; Pruyt 2007). System dynamics is traditionally used for modeling and simulating dynamically complex issues, analyzing the resulting non-linear behaviors over time, and developing and testing structural policies. Most dynamically complex problems are characterized by deep uncertainty, since in case of dynamic complex issues the cause effect relations are subtle (Senge 1990). The omnipresence of uncertainty has been recognized by many system dynamicists and is the underlying motivation for interpreting the quantitative results of system dynamics models qualitatively (e.g. in term of modes of behaviors or behavioral trajectories) (Meadows and Robinson 1985; Pruyt 2007). This qualitative interpretation of model results is compatible with the interpretation of model results in EMA.

Two basic search strategies exist in the context of EMA: open exploration and directed search. Open exploration can be used to systematically explore the set of plausible models. This exploration relies on the careful design of the computational experiments and can use techniques such as Monte Carlo sampling, Latin Hypercube sampling, or factorial methods. An open exploration can be used to answer questions such as "What kind of behavioral trajectories can the system exhibit?" "Under what circumstances would this policy do well? Under what circumstances would it likely fail?" An open exploration provides insight into the full richness of behaviors that the ensemble of models can exhibit. Coupled with various analytic techniques, such as rule induction methods, an open exploration can also reveal the necessary conditions for the occurrence of a particular behavior, or the success of failure of policies. Directed search, in contrast, is a search strategy for finding particular cases that are of interest. Directed search can be used to answer questions such as "What is the bandwidth of model outcomes over time?" "what is the worst that could happen?" What is the best that could happen?" "How big is the difference in performance between rival policies?". A directed search provides detailed insights into the dynamics of specific locations in the full space of plausible models. Directed search relies on the use of optimization techniques, such as genetic algorithms and conjugant gradient methods. Active non-linear test are an example of a directed search strategy (Miller 1998). Open exploration and directed search can complement each other. For example, if the open exploration reveals that there are distinct regions of possible dynamics, directed search can be employed to identify more precisely where the boundary is located between these distinct regions.

2.3 An optimization algorithm for directed search

A suitable optimization algorithm for directed search in the context of System Dynamics models should be able to cope with the non-linearity of the model, a non-linear objective function, discontinuities in the search space, a search space that is rife with local optima, and noise (Miller 1998). In the context of EMA, two additional complications are added, namely a potentially very large search space, and a discontinuous search space arising out of the inclusion of variations in e.g. structural equations. On top of this, a suitable optimization algorithm should be economical. That is, it should be able to find the optimum relatively quickly, without requiring a very large number of computational runs. As argued by Miller (1998), Genetic Algorithms (GA) are a perfect candidate that is able to meet the outlined requirements.

GA have proved to be an effective optimization algorithm for complex optimization problems (Goldberg 1989) due to their flexibility and efficiency in complex and irregular solution spaces (Chambers 1999). GA is inspired by the process of natural selection observed in biological systems (Fraser and Burnell 1970; Holland 1975). A GA starts with a population of randomly generated candidate solutions characterized by their model parameters. Each member of this population is a chromosome. And each chromosome consists of a alleles. Each allele corresponds to a particular model parameter. The fitness of the fitness of each population member of the initial population is assessed using a user specified objective function. In light of the fitness scores of the current population members, a next generation is created. The next generation is created , through evolutionary processes such as mutation and crossover . Mutation randomly makes alterations in candidate solutions. In crossover, more than one member from the previous generation are recombined into a member of the next generation. Once the next generation is created, the fitness calculations are computed again for the new population members. This process of fitness evaluation and reproduction of new generation is repeated until a pre-specified termination criterion is met. Possible termination criteria include reaching a desired solution, a fixed number of iterations, and convergence of the fitness scores.

3 ANEMI

ANEMI, an ancient Greek term for the four winds, heralds of the four seasons, links physical systems such as climate, the hydrological cycle and the carbon cycle with socio-economic systems, including economy, land use, population change and water use (Davies and Simonovic 2010). It was designed as an integrated assessment model that would permit the assessment both of socio-economic policies and uncertainties about the overall system (Davies and Simonovic 2010). ANEMI is a system dynamics model, focusing in particular on the importance of the feedback relations between the various physical and socio-economic subsystems, and the dynamics arising out of these feedbacks, rather than aiming at providing detailed predictions.

ANEMI is a System Dynamics model. Central to System Dynamics models is the endogenous point of view (Richardson 2011). According to this view, the dynamic behavior of a system arises within the internal structure of a model. This view implies a closed system boundary, where the behavioral dynamics of the system arise out of interacting feedback loops. Thus, in System Dynamics, a system is viewed as an ongoing interdepended, self-sustaining, dynamic process. That is, the observed behavior of a system is to be understood as arising out of the internal structure of the system. This internal structure of a system is conceptualized using stocks and flows, and relations between them. System Dynamics is a modeling method for understanding the behaviors of nonlinear, dynamic and complex systems and for policy analysis and design (Sterman 2000).

ANEMI is composed of nine subsystems: climate, carbon cycle, economy, land-use, population, agricultural production, natural hydrological cycle, water use, and water quality (Davies 2007; Davies and Simonovic 2008, 2011). Figure 1shows the main feedback structure of the model. The positive or negative sign associated with each arrow indicates the direction of change one model component has on the other model component. The names next to each arrow indicate which aspect of the model component causes a change in the other model component. The closed loop structure of the model implies that model behavior emerges endogenous feedbacks (Davies and Simonovic 2010). The model has been validated through comparison with government statistics, scientific data, results from other models, and socio economic data (Davies 2007; Davies and Simonovic 2008, 2010, 2011).

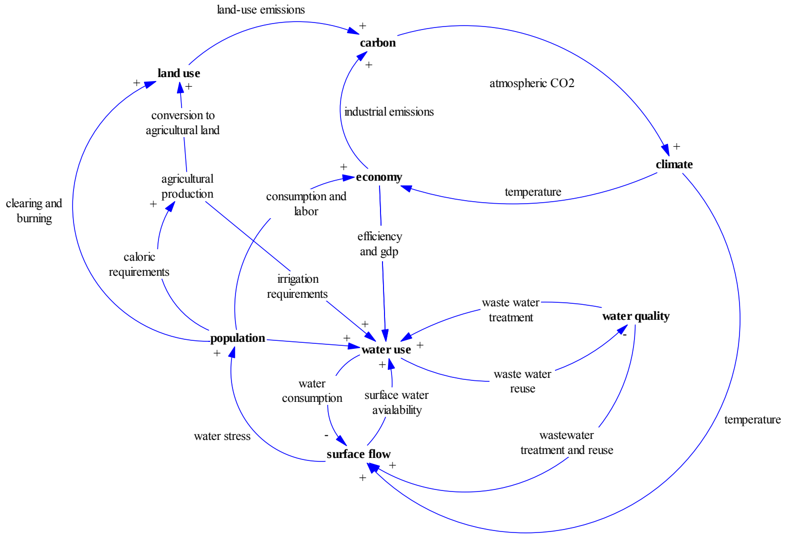

Figure 1: Model components and their feedbacks (Davies and Simonovic, 2011)

The climate sector is an upwelling diffusion energy balance model based on the box advection diffusion model of Harvey and Schneider (1985). The carbon cycle is based on Goudriaan and Ketner (1984), where the oceanic sector is modified based on Fiddaman (1997). The land use system is based on Goudriaan and Ketner (1984). The population component is based on Nordhause and Boyer (2000) and Fiddaman (1997). However, the dynamics are endogenous by including water stress (Davies and Simonovic 2010). The economic components is inspired by the updated DICE model (Nordhaus 2008). The three water parts and the agricultural production are unique to ANEMI, but build on earlier work (e.g. Shiklomanov 2000; Simonovic 2002). The water use model is similar to WaterGAP 2 (Alcomo et al. 2003). Water quality is comparable to how it is handled in WorldWater (Simonovic 2002). Surface flow, and the hydrological cycle are influenced by Chanine (1992), Shiklomanov (2000), and Simonovic (2002). The agricultural component is the latest addition to ANEMI and is based on Bouwman et al. (2005), Siebert and Döll (2010), and FAO data (Davies and Simonovic 2011). ANEMI is implemented in Vensim (Ventana Systems Inc. 2011).

4 Results

4.1 Defining the search space

Table 1 contains an overview of the parameters and their ranges that constitute the search space. For this paper, we concentrated on parameters related directly to water use. The documentation of the model was reviewed and parameters that were either explicitly denoted as a guess or assumption, or for which divergent possible values were named, were included in the analysis. The parameters include various time series that describe developments over the full runtime, such as the changing demand for food per person per year. These time series were replaced with sigmoid functions:

$$f(t) = \alpha \frac{1}{1 + e^{\frac{t-\gamma}{\delta}}} + \beta$$

Here, α, β, γ, δ, are uncertain parameters that can be explored; α and β control the upper and lower limit of the sigmoid, γ controls when the sigmoid is half way between the two limits, and δ controls the slope. In this way, structural uncertainty related to the parameterization of table functions is included in the analysis.

Table 1. The uncertainties and their ranges

uncertainty	description	range
Agricultural Blue Water Dilution Factor	factor for dilution of polluted agricultural blue water	5-10
Agricultural Polluted Fraction	percentage of return flow of agricultural blue water that is polluted	0.7-0.95
Average Virtual Water Content of Crops	virtual water in crops in m3/Gcal	400-500
Average Virtual Water Content of Fodder	virtual water in fodder in m3/Gcal	200-300
Base Specific Water Intake	base value for water intake in agriculture in m3/ha/year	9000-12000
Base Returnable Water	base value for water return flow from agriculture in m3/ha/year	10-50
Base Precipitation Multiplier	increase of precipitation due to increasing global temperature in %/Celsius	3-4
Domestic Dilution Factor	factor for dilution of polluted domestic water	5-10
Domestic Polluted Fraction	percentage of return flow of domestic water that is polluted	90-100
Fractional Usage of Desalination Capacity	fraction of desalinization capacity that is being used	0.3-0.7
Fcl	simple area weighted cloud fraction	0.5-0.6
Gamma d	factor affecting increase in water demand per person due to gdp/capita increase	2.2e-10-2.2e-06
Industrial Dilution Factor	factor for dilution of polluted industrial water	5-10
Industrial Polluted Fraction	percentage of return flow of industrial water that is polluted	38-46
Max Groundwater Withdrawal	maximum amount of ground water withdrawal in km3/Year	7-10
Maximum Establishment of Desalination Facilities	maximum amount of desalinization capacity in km3/year	25-40
Percent Domestic Withdrawal	percentage of domestic withdrawal that is consumed	80-90
Stable and Useable Runoff Percentage	fraction of runoff that can be used, taking pollution dilution into account	30-40
Yield Ratio for rainfed to irrigated agriculture	yield fraction of rain fed agriculture as compared to irrigated agriculture	0.4-0.8
Wastewater Dilution Requirement	multiplier for dilution of polluted water	6-10

Technological Change for Consumption in Agricultural Sector lookup	transient scenario for technological change in agriculture affecting water consumption	sigmoid function
Technological Change for Withdrawals in Agricultural Sector lookup	transient scenario for technological change in agriculture affecting water withdrawal	sigmoid function
Crop Productivity Gains lookup	transient scenario for gains in crop productivity	sigmoid function
Percentage increase in irrigated area lookup	transient scenario for increase in irrigated area	sigmoid function
Global Per Capita Food Consumption lookup	transient scenario for increase in food consumption	sigmoid function

In order to explore the behavior of the model over the listed uncertainties, a shell written in Python is utilized. This shell is used for our convenience only, and not because of the fact that existing System Dynamics software does not allow for performing EMA. This 'EMA workbench' controls Vensim through its Dynamic Link Library (DLL). The workbench is responsible for generating input values for the various uncertainties, setting these values on the models, executing the models, and storing its results. The workbench supports parallel processing to reduce computational time. The genetic algorithm was based on the open source library PyEvolve, which was extended to fit into the overall architecture of the EMA workbench.

4.2 Application of GA

Two separate optimizations are executed. We maximize the water stress over the run and we minimize the terminal value for the world population. Water stress is an indicator of the fraction of renewable water that is being used on a yearly basis. Typically, values higher than 0.4 are labeled as severe water stress and indicate potential local or regional shortages and water related conflicts (Alcomo, Flörke, and Märker 2007). A value for water stress well above 0.4 over the run thus indicates that a limit to fresh water usage has been passed (Alcomo et al. 2003). Given that the idea of planetary limits is closely tied to the thriving of human civilization and the world's population, looking at the lowest value for the world population in 2100 is a good proxy for having passed a limit to fresh water use. Thus, we look at two different ways of understanding limits to the planetary fresh water cycle.

The GA was parameterized as follows. Each generation contained a 1000 population members. We ran the optimization for 100 generations, with a crossover rate of 0.01 and a mutation rate of 0.05. That is, there is a 1% chance for a random mutation for each population member and a 5% change of a crossover when creating the next generation. Figure 2 shows the evolution of the algorithm over the generations for maximizing the water stress. The line indicates the average score on the objective function, and the error bars indicate the minimum and maximum value encountered in each generation. As can be seen, the algorithm converged after roughly 60 generations. For the minimization of the world population in 2100, a similar figure emerges.

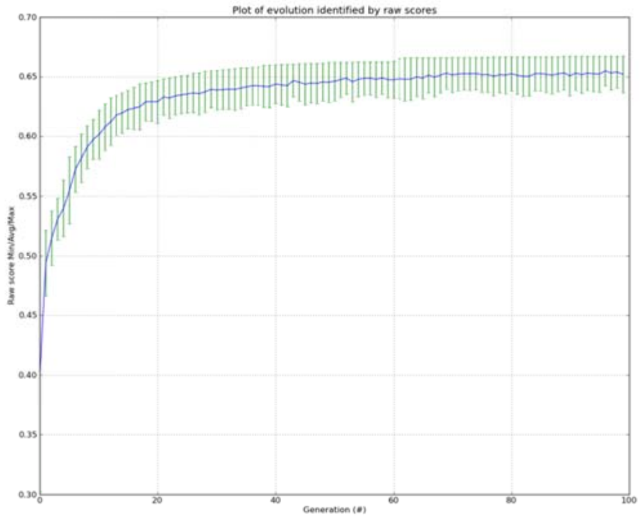

Figure 2: Convergence of the maximization of the water stress

Table 2 shows the results found using the GA. Not surprisingly, the water stress is maximized in the case that has the highest value for beta food consumption (the terminal value for the sigmoid function that describes the change in food demand per person over time). Surprisingly, the highest water stress is reached when the dilution requirements for the return flow from the various usages of water is low. That is, both the dilution factor and the polluted fraction for both domestic use and industrial use are at the low end of the range. A possible explanation for this is that a slow buildup of water stress over time results in a higher maximum value for the water stress. This explanation is supported by comparing the two cases. As can be seen in Figure 3, the water stress builds up much slower for the maximum water stress case as compared to the lowest world population.

Table 2: The parameterizations found using the GA

	maximum water stress	minimum world population
Agricultural Blue Water Dilution Factor	9.996741712	5.975799095
Agricultural Polluted Fraction	0.945110585	0.757602212
alpha crops	2.000460806	2.025001173
alpha food consumption	1501.757554	1831.893768
alpha irrigated area	0.399317149	0.384175296
Average Virtual Water Content of Crops	445.2044613	430.2811226
Average Virtual Water Content of Fodder	261.5618128	207.167041
Base Precipitation Multiplier	3.995920224	3.235194036
Base Returnable Water	10.06048083	36.17342705
Base Specific Water Intake	11986.998	11992.27777
beta consumption	0.895189296	0.729342246
beta crops	0.000943524	0.089050287

beta food consumption	3499.264192	3450.646339
beta irrigated area	2.492830323	2.354092042
beta withdrawals	0.500340128	0.833152332
delta consumption	14.20058734	29.47769271
delta crops	29.87094202	28.23127418
delta food consumption	29.94513384	10.21213091
delta irrigated area	39.78929775	28.99601442
delta withdrawals	10.00156791	21.76345533
Domestic Dilution Factor	5.011686103	9.824745751
Domestic Polluted Fraction	90.00941738	97.17528749
Fcl	0.599431203	0.591478507
Fractional Usage of Desalination Capacity	0.698533655	0.585355964
gamma consumption	2000.160573	2069.071024
gamma crops	2009.940357	2009.57812
Gamma d	4.56E-09	1.25E-06
gamma food consumption	1959.857032	1941.496592
gamma irrigated area	1999.999505	1998.977764
gamma withdrawals	2047.942128	2001.943708
Industrial Dilution Factor	5.007851723	9.196068032
Industrial Polluted Fraction	38.0476917	39.11256461
Max Groundwater Withdrawal	7.100233952	7.465027144
Maximum Establishment of Desalination Facilities	39.86164451	37.64254459
Percent Domestic Withdrawal	80.01281784	86.7731994
Stable and Useable Runoff Percentage	34.9647949	32.61353969
Wastewater Dilution Requirement	9.638636676	8.499785182
Yield Ratio for rainfed to irrigated agriculture	0.400061095	0.403879995

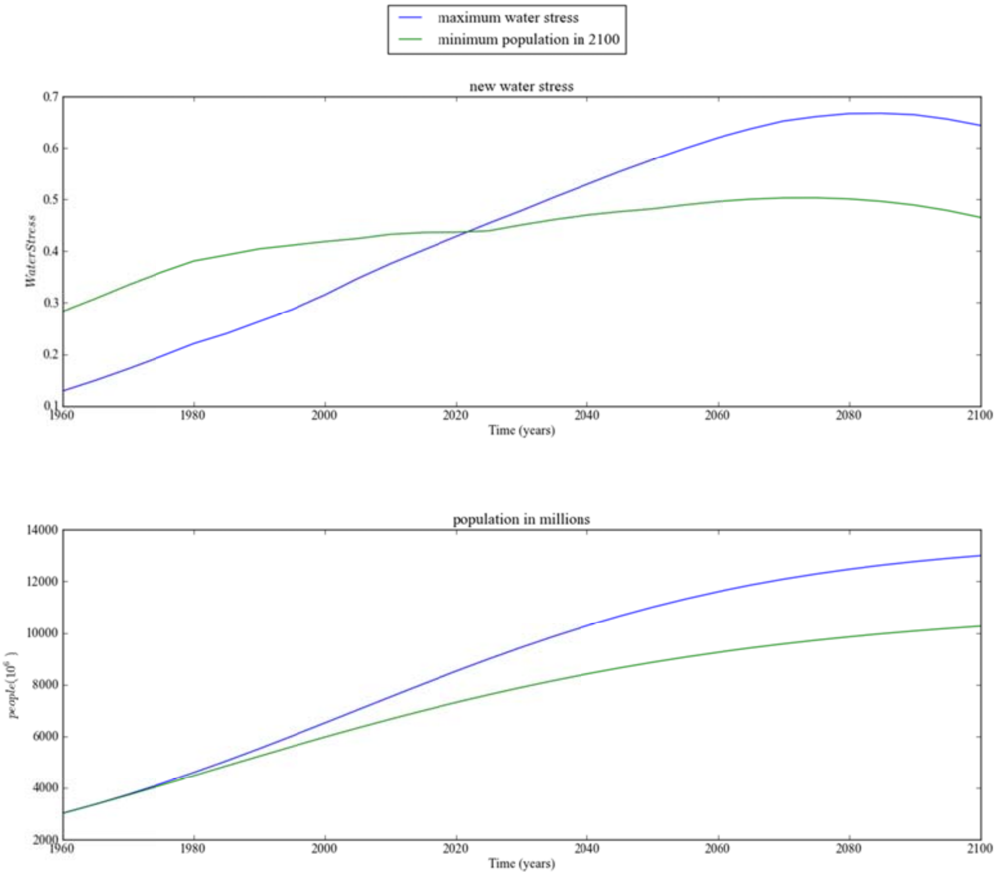

Figure 3: Dynamics for the size of the world population and water stress for both the maximum water stress and minimum population in 2100.

5 Closing Remarks

The model considered in this paper is an integrated dynamic model of the world water cycle, taking into consideration the climate system, the population system, the economic system etc. However, this integration comes at the price of being not geographically and temporally explicit. Thus, changes in geographic precipitation patterns or shifts in the seasonal rain patterns are not included in this model. Still, the result indicate that even with modest bandwidth on several water cycle related parameters, the model can already produce results that are indicative of severe water stress or limited growth of the world population. As such, our results indicate that even at a high level of aggregation, planetary limits to the fresh water cycle develop and can be investigated.

Our results do not translate to limits. We only identified two cases with undesirable dynamics: a low value for the world population and a very high value for water stress. It remains an open question how to relate these results to limits. One obvious way of understanding limits is in terms of overshoot and decline dynamics. For water stress, the maximum value falls after reaching its maximum, thus suggesting the presence of overshoot and decline dynamics, and thus the presence of a limit, in this case. An open exploration could be used to investigate this further. The aim of such an investigation would be to identify the subspace of parameterizations of the model that produces this dynamic and the feedback loops responsible for the decline.

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