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Sincerely,

Peter Sandborn
Director of Graduate Studies
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Sincerely,

Steven A. Gabriel

Steven Gabriel
Advisor for Nathan Boyd

ABSTRACT

Title of Dissertation: EQUILIBRIUM PROGRAMMING FOR IMPROVED MANAGEMENT OF WATER-RESOURCE SYSTEMS

Nathan T. Boyd
Doctor of Philosophy, 2024

Dissertation Directed by: Professor Steven A. Gabriel
Department of Mechanical Engineering

Effective water-resources management requires the joint consideration of multiple decision-makers as well as the physical flow of water in both built and natural environments. Traditionally, game-theory models were developed to explain the interactions of water decision-makers such as states, cities, industries, and regulators. These models account for socio-economic factors such as water supply and demand. However, they often lack insight into how water or pollution should be physically managed with respect to overland flow, streams, reservoirs, and infrastructure. Conversely, optimization-based models have accounted for these physical features but usually assume a single decision-maker who acts as a central planner.

Equilibrium programming, which was developed in the field of operations research, provides a solution to this modeling dilemma. First, it can incorporate the optimization problems of multiple decision-makers into a single model. Second, the socio-economic interactions of these decision-makers can be modeled as well such as a market for balancing water supply and de-

mand. Equilibrium programming has been widely applied to energy problems, but a few recent works have begun to explore applications in water-resource systems. These works model water-allocation markets subject to the flow of water supply from upstream to downstream as well as the nexus of water-quality management with energy markets.

This dissertation applies equilibrium programming to a broader set of physical characteristics and socio-economic interactions than these recent works. Chapter 2 also focuses on the flow of water from upstream to downstream but incorporates markets for water recycling and reuse. Chapter 3 also focuses on water-quality management but uses a credit market to implement water-pollution regulations in a globally optimal manner. Chapter 4 explores alternative conceptions for socio-economic interactions beyond market-based approaches. Specifically, social learning is modeled as a means to lower the cost of water-treatment technologies.

This dissertation's research contributions are significant to both the operations research community and the water-resources community. For the operations research community, this dissertation could serve as model archetypes for future research into equilibrium programming and water-resource systems. For instance, Chapter 1 organizes the research in this dissertation in terms of three themes: stream, land, and sea. For the water-resources community, this dissertation could make equilibrium programming more relevant in practice. Chapter 2 applies equilibrium programming to the Duck River Watershed (Tennessee, USA), and Chapter 3 applies it to the Anacostia River Watershed (Washington DC and Maryland, USA).

The results also reinforce the importance of the relationships between socio-economic interactions and physical features in water resource systems. However, the risk aversion of the players acts as an important mediating role in the significance of these relationships. Future research could investigate mechanisms for the emergence of altruistic decision-making to improve equity among the players in water-resource systems.

EQUILIBRIUM PROGRAMMING FOR IMPROVED MANAGEMENT OF WATER-RESOURCE SYSTEMS

by

Nathan T. Boyd

Dissertation submitted to the Faculty of the Graduate School of the
University of Maryland, College Park in partial fulfillment
of the requirements for the degree of
Doctor of Philosophy
2024

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To my son Jackson: I hope one day this work will inspire you to hone your own interests and to find a positive outlet to share them with others.

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In Memory of: my maternal grandfather Howard Brooks Sims Jr. (1924 - 2024). Your belief in using reason to make a better world is reflected in the spirit of this work.

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List of Abbreviations

BMP	Best Management Practice
CAST	Chesapeake Assessment Scenario Tool
CBWM	Chesapeake Bay Watershed Model
CDF	Cumulative Distribution Function
CSM	Cost-Sharing Market
CVaR	Conditional Value at Risk
DRUC	Duck River Utility Commission
ESB	Earth-System Boundary
EV	Electric Vehicle
GCM	General Commodity Market
HSPF	Hydrological Simulation Program Fortran
KKT	Karush-Kuhn-Tucker Optimality Conditions
KS1	1-Sample Kolmogorov–Smirnov
LCP	Linear Complementarity Problem
MC	Montgomery County
MCP	Mixed Complementarity Problem
MGD	Million Gallons per Day
MIP	Mixed Integer Linear Program
MPEC	Mathematical Program with Equilibrium Constraints
NE	Nash Equilibrium
NEB	Northeast Branch
OR	Operations Research
PG	Prince George's County
ROI	Return on Investment
SAV	Submerged Aquatic Vegetation
SOS1	Special Ordered Set Type 1
ST	Sustainability Transitions
SysML	Systems Modeling Language
TCMD	Thousand Cubic Meters per Day
TMDL	Total Maximum Daily Load
WY	Water Year

Chapter 1: Introduction

1.1 Motivation

Water-resources management inevitably involves the socio-economic interactions of many decision-makers. One reason for the multiplicity of these interactions is the scale of water usage. An astonishing 4,600 cubic kilometers of water is used for human purposes [2]. In the natural world, freshwater habitats contain 10 % of earth's species [3]. Another reason is the transboundary nature of water. 60 % of the world's rivers, lakes, and aquifers span multiple countries [4]. Therefore, understanding these socio-economic interactions is necessary to understand how water resources are managed.

Ultimately, hydrology and infrastructure create the central issues inherent to these interactions. Recent hydropower projects on the Nile and Mekong rivers have raised issues about how flow should be maintained fairly between upstream and downstream water users [5]. In the Colorado River Basin, a severe drought is forcing the renegotiation of a century-old agreement for water allocations [6]. In terms of water quality, natural landscapes have been transformed into urban and agricultural land, degrading natural ecosystems in the process [4].

Knowledge transfer from one geographic niche to another also presents opportunities for water decision-makers to interact. The city of Windhoek, Namibia satisfies 25 % of its water demand using wastewater reuse because it is arid and too far from the ocean to adopt desalination.

Water managers in the Mediterranean face similar challenges and could benefit from knowledge transfer from the Windhoek setting [7]. More globally, only 11 % of wastewater is reused leaving the potential to generate roughly 320 billion cubic meters of recycled water per year [8].

Thus, water management decision models need to account for 1) multiple decision-makers and 2) the physical characteristics of water. These characteristics include: hydrology, infrastructure, and local geography. Despite this need, mathematical models considering these aspects in detail have been rare. Mathematical optimization models have considered these physical characteristics but typically with a single decision-maker [9] or sequential decision-makers [10]. Similarly, game theory has been used to model multiple water decision-makers while neglecting physical characteristics [11] [12].

1.2 Modeling Approach

Despite these trends, a few seminal papers with multiple decision-makers and detailed physical characteristics explore issues related to water allocation [13] [14] [15] [16], water quality [17], and nutrient recovery from wastewater [18] [19] [20]. In these works, each decision-maker optimizes a dedicated mathematical program with constraints related to water quantity and/or quality characteristics. Other constraints quantify how the decision-makers interact. For example, the decision-makers could trade water rights in a market.

In most of these seminal papers, each decision-maker, denoted as player $p \in P$, solves a mathematical program of the following form:

$$\min f_p(x_p) \tag{1.1a}$$

s.t.

$$g_{p,i}(x_p) \leq 0 \quad , \quad i = 1, ..., m_1^p \quad (u_{p,i}) \tag{1.1b}$$

$$h_{p,j}(x_p) = 0 \quad , \quad j = 1, ..., m_2^p \quad (v_{p,j}) \tag{1.1c}$$

Player p's set of decision variables is given by $x_p \in \Re^{n_p}$ [1]. The objective function f is convex as is the constraint function g. The constraint function h is affine. The variables u and v are Lagrange multipliers.

Consider the following simple example of a water system that could be modeled using (1.1). Player p could be a municipality trying to minimize water-supply costs. The function g could represent water demand minus water supply. The function h could represent the mass balance of water flowing from upstream to downstream. The multipliers could represent the cost savings associated with a small increase in water supply.

Program (1.1) can be re-expressed via the Karush-Kuhn Tucker (KKT) optimality conditions [21]:

For each $p \in P$, find the vectors $\bar{x}_p, \bar{u}_p, \bar{v}_p$ s.t.:

$$\nabla f_p(\bar{x}_p) + \sum_{i=1}^{m_1^p} \bar{u}_{p,i} \nabla g_{p,i}(\bar{x}_p) + \sum_{j=1}^{m_2^p} \bar{v}_{p,j} \nabla h_{p,j}(\bar{x}_p) = 0 \tag{1.2a}$$

$$g_{p,i}(\bar{x}_p) \leq 0 \quad , \quad \bar{u}_{p,i} \geq 0 \quad , \quad g_{p,i}(\bar{x}_p) \perp \bar{u}_{p,i} \quad , \quad i = 1, ..., m_1^p \tag{1.2b}$$

$$h_{p,j}(\bar{x}_p) = 0 \quad , \quad \bar{v}_{p,j} \quad free \quad , \quad j = 1, ..., m_2^p \tag{1.2c}$$

[1] The terms n_p,m_1^p, and m_2^p are positive integers that are problem specific.

where $g_{p,i}(\bar{x}_p) \perp \bar{u}_{p,i} \equiv \bar{x}_p \bar{u}_{p,i} = 0$. The convexity assumptions of f and g as well as the affine assumption of h make these KKT conditions sufficient for an optimal solution to Program 1.1 [22].

Additional system constraints, such as market-clearing conditions, are used to govern the interactions among the players. To represent these mathematically, consider an q-dimensional [2] system of equations of the following form:

$$\Gamma_k(x) = 0 \quad , \quad \pi_k^{sys} \quad free \quad , \quad k = 1, ..., q \quad , \quad x = [x_1^T, ..., x_{|P|}^T]^T \tag{1.3}$$

Expression 1.3 can also represent inequalities without loss of generality via the use of slack variables.

In words, let Γ be a function that determines some additional vector π^{sys}. This function takes the union of all the player's decisions as an argument. Crucially, the components of π^{sys} are not decision variables in (1.1) for any player p. However, they can represent parameters that the players must consider in their optimization problems. For example, π_k^{sys} could represent the price to remove water pollutant k (e.g., nutrients, sediment, etc.). In this context, the players accept the prices as given and don't try to manipulate them.

Combining (1.2) and (1.3) generates a system of equations where all the nonlinear terms are complementarity expressions (i.e., the $\perp$ operator). A solution to this system is not necessarily system optimal because each player solves their optimization problem individually. Rather, a solution is called an equilibrium solution because it emerges from the interaction of the players. For this reason, the system of (1.2) and (1.3) is a specific and common manifestation of an

[2] q is a positive integer that is problem specific.

equilibrium program.

Equilibrium programming has also been used to provide economic-policy insights for other energy and natural resource systems such as electric power or natural gas. It contextualizes the role of spatial and temporal features of supply and demand. Market failures in liberalized electric power and natural gas systems have been attributed to a lack of understanding of these features [23]. Thus, the research in this thesis aims to replicate the successes of electric power and natural gas liberalization in water systems while avoiding some of the failures.

1.3 Overview of Thesis Projects

This dissertation features three projects applying equilibrium programming to water management problems (Figure 1.1). Each project has a dedicated chapter and a theme. Chapter 2 focuses on the flow of water from upstream to downstream. In contrast, Chapter 3 focuses on the flow of water over land surfaces as well as pollution sources like nitrogen and sediment. Lastly, Chapter 4 focuses on alternatives to freshwater that are very abundant but are difficult to treat for human use (e.g., seawater).

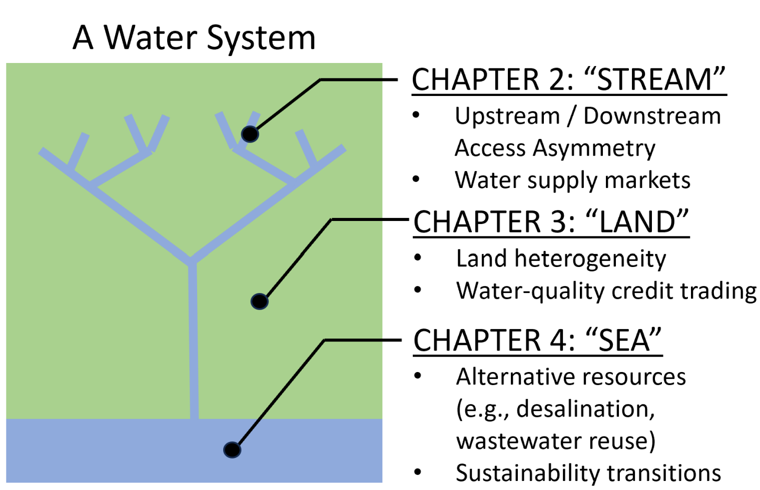

Figure 1.1: Dissertation project themes

Each chapter explores how the theme of interest brings multiple water decision-makers into interaction. Chapter 2 explains how a water-supply market could emerge to improve downstream users' access to water. In Chapter 3, management jurisdictions trade credits to coordinate the reduction of water pollution from heterogeneous land areas (e.g., urban vs. rural). In Chapter 4, population centers invest in advanced water-treatment technologies (e.g., seawater desalination). These investments may secure an abundant supply of water to help transition away from the unsustainable depletion of freshwater.

As described in Section 1.2, player $p \in P$ solves a convex optimization problem. In Chapter 2, the players each solve convex quadratic programs. In Chapter 3, the players solve non-linear, convex programs that have second-order-cone constraints. In Chapter 4, all but one player solve linear, stochastic programs. The remaining player solves a non-convex optimization problem called a mathematical program with equilibrium constraints. This special player serves as policymaker who takes the actions of the other players into account.

In some cases, the equilibrium programs in this dissertation have zero or multiple solutions. In Chapter 2, the computation of the water-supply market equilibrium prices varied according to the starting values provided to the solver. In Chapter 3, zero solutions were possible (i.e., problem was infeasible), when the pollution-reduction targets exceeded the effectiveness of the technologies available to reduce water pollution. In Chapter 4, multiple solutions were possible but these occurred at discontinuities in piecewise linear cost curves.

Two testbeds are considered as a part of these research projects. The Duck River Watershed is the testbed in Chapter 2. It is located in middle Tennessee south of Nashville. Recent population growth in the region has accentuated the need to provide adequate urban water supplies without compromising aquatic biodiversity. The Anacostia River Watershed is the testbed in

Chapter 3. It is located in Washington, DC and Maryland. This is a historically urban watershed that is being restored to meet water quality standards.

Stakeholders from the Duck and Anacostia River testbeds provided their feedback on the models in Chapters 2 and 3, respectively. This feedback was elicited from presentations given during the Duck River Development Agency Technical Advisory Committee Meeting and two workshops held in Washington, DC. The details for these presentations are described in Section 1.5. In general, the stakeholders were receptive to the new socio-economic norms (e.g., optimization problems, market structures) obtained from these models.

The stakeholders' positive feedback represents a key step towards real-world verification of the Chapter 2 and 3 models, but much work remains. Fundamentally, the socio-economic norms in this dissertation describe the world as it could be instead of the *status quo*. Therefore, real-world implementation of these norms is necessary for true verification. Endorsements from federal, state, and local policymakers are crucial because they can establish a legal basis for these water-management norms. Much work remains to obtain this policymaker buy-in.

Several stylized examples also appear in these research projects. These examples are not based on real-world locations but accentuate general features of their corresponding mathematical models. In Chapter 2, a series of three-player examples are developed to compare two water-market designs. In Chapter 3, a stylized example is used to illustrate model features. Chapter 4 relies solely on a stylized water-resources example. This project is more conceptual than the others because it emphasizes a general model that could be applied to multiple natural-resource contexts.

These stylized examples reveal opportunities and challenges associated with broad application of this dissertation's models. In Chapters 2 and 3, the stylized examples could help identify new testbeds beyond the Duck and Anacostia Rivers. For example, the three-player examples in Chapter 2 could be mathematically like any number of real-world watersheds. In Chapter 4, the stylized model reveals the difficulty of estimating cost scenarios for advanced water-treatment technologies. These estimates would likely depend on subjective, expert judgements, which are inherently difficult to verify objectively.

1.4 Selected Insights

Despite these verification challenges, the models in this dissertation test water-resource-related policies in a virtual environment prior to real-world implementation. This testing is beneficial because anticipating the full implications of a policy in a water-resource system with many interacting decision-makers and complex hydrological processes would be extremely challenging. Surprising model results aid decision-makers in better understanding these implications. Doing so could then help account for potential unintended real-world consequences. Depending on the context, these unintended consequences could be either positive or negative. Positive unintended consequences could be capitalized upon, while negative unintended consequences could be avoided. Thus, with this in mind, this section presents selected insights from the subsequent chapters that are both positive and negative.

In Chapter 2, two unintended consequences were identified: one negative and one positive. The negative consequence is that profits in the water-supply market increased water consumption overall, which countered water-efficiency improvements somewhat. The positive consequence is, however, for all the cases tested, there was a market design that was overall more favorable than having no market at all.

Table 1.1: List of papers associated with this dissertation

Paper Title	Chapter	Status	Next Steps	Target Date	Lead?	Co-authors
Generalized Nash equilibrium models for asymmetric, non-cooperative games on line graphs: Application to water resource systems [24]	2	Published in *Computers and Operations Research*	N/A	N/A	Y	Steven Gabriel, George Rest, Tom Dumm
Inverse Optimization for Parameterization of Linear Complementarity Problems and for Incentive Design in Markets [25]	2	In Preparation	Revise	08/24	N	Stephanie Allen, Steven Gabriel
Reducing Pollution in River Systems using a Stochastic, Game-Theoretic Modeling Approach [26]	3	Submitted	Pending	Pending	Y	Steven Gabriel, Kaye Brubaker, Matthew Ries
Understanding the Role of Technological Complexity in Water-Resource Transitions using Stochastic, Bi-level Optimization [27]	4	Submitted	Pending	Pending	Y	Steven Gabriel

In Chapter 3, there was a surprising result related to the prices and investments in the credit-trading market. Specifically, a nearly mutually-exclusive relationship was discovered in the investment trade-offs for eliminating two forms of water pollution: wash-off sediment and nitrogen. This emphasized the importance of investments that reduce multiple forms of water pollution simultaneously and suggests that the model could be solved more efficiently by being decomposed into subproblems. In terms of policy, this suggests that detailed models are needed to best understand which forms of water pollution (e.g., wash-off sediment, nitrogen) are the most difficult forms to mitigate.

1.5 Papers and Presentations

The results of this dissertation are disseminated in several papers and many presentations. Table 1.1 summarizes the papers associated with this dissertation. This table includes the corresponding dissertation chapter, status, next steps, dates, and lead author designation. Similarly, Table 1.2 summarizes the presentations. This table includes the title, associated chapter, conference name and date, status, and presentation role.

Table 1.2: Presentations accompanying this dissertation

Presentation Title	Chapter	Organizer/Conference	Location	Status	Date	Lead?	Co-presenters
Modeling Water-Use Benefits and Risks in the Duck River Watershed	2	Duck River Development Agency Technical Advisory Committee Meeting	Virtual	Presented	10/12/2021	Y	Steven Gabriel
Game Theoretic Modeling For Improved Management Of Water And Wastewater Resources Using Equilibrium Programming And Feedback Mechanisms	2	INFORMS Annual Meeting 2021	Anaheim, CA	Presented	10/24/2021	Y	Steven Gabriel, George Rest, Tom Dumm, Doug Murphy
Water Resources Equilibrium Programming	2	Trans-Atlantic Infraday 2021	Espoo, Finland	Presented	11/11/2021	Y	Steven Gabriel, George Rest, Tom Dumm
Alternative TMDL Allocation Schemes using Game-Theoretic Modeling	3	American Water Resources Association (AWRA), National Capital Region Conference 2022	Washington, DC	Presented	4/8/2022	Y	Steven Gabriel, Kaye Brubaker, Matt Ries
Generalized Nash Equilibrium Models for Asymmetric River Systems	2	European Conference on Stochastic Optimization, Computational Management Science ECSO-CMS 2022	Venice, Italy	Presented	6/29/2022	N	Steven Gabriel
Anacostia River Stakeholder Meeting: Game Theory Modeling and Market Theory for Water Management	3	DC Water	Washington, DC	Presented	10/27/2022	Y	Steven Gabriel, Kaye Brubaker, Matt Ries, Stephanie Allen
Inverse Optimization for Parameterization of Linear Complementarity Problems and for Incentive Design in Markets [25]	2	Trans-Atlantic Infraday 2022	Stockholm, Sweden	Presented	11/3/2022	N	Stephanie Allen, Steven Gabriel
Can Game Theory Improve Water-Quality Restoration Decisions?	3	Trans-Atlantic Infraday 2022	Stockholm, Sweden	Presented	11/3/2022	Y	Steven Gabriel, Kaye Brubaker, Matt Ries
Envisioning Water-Resource Transitions using Complexity Science	4	Santa Fe Institute 2023 Graduate Workshop in Computational Social Science	Santa Fe, NM	Presented	6/29/2023	Y	N/A
Equilibrium Problems Applied to Water Markets	3	Trans-Atlantic Infraday 2023	Paris, France	Presented	11/9/2023	N	Steven Gabriel
Second Workshop on Use of Game Theory Modeling and Market Theory for Water Management	3	DC Water	Washington, DC	Presented	1/30/2024	Y	Steven Gabriel, Kaye Brubaker, Matt Ries
Reducing Pollution in River Systems using a Stochastic, Game-Theoretic Modeling Approach	3	World Environmental and Water Resources Congress 2024	Milwaukee, WI	Presented	5/21/2024	Y	Matt Ries, Steven Gabriel, Kaye Brubaker
Reducing Pollution in River Systems using a Stochastic, Game-Theoretic Modeling Approach	3	AWRA Joint Water Resources Conference 2024	St. Louis, MO	Upcoming	9/30/2024	TBD	Kaye Brubaker, Steven Gabriel, Matt Ries
Allocation Policies Involving Finite and Practically Unlimited Resources	4	Trans-Atlantic Infraday 2024	Rio de Janeiro, Brazil	Upcoming	10/31/2024	Y	Steven Gabriel

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Chapter 2: Generalized Nash equilibrium models for asymmetric, non-cooperative games on line graphs: Application to water resource systems

2.1 Introduction

2.1.1 Asymmetric Games

In engineering-economic and other systems, asymmetric games exist if some players have distinct advantages over other players. These advantages may be structural, e.g., first-mover advantage , e.g. Stackelberg games [21] or may take the form of disproportionately higher payoffs, a greater number of strategies, or other aspects. Concerns regarding equity and welfare arise when these situations involve shared resources or infrastructure of economic, social, or environmental importance. Thus, ways to balance this asymmetry provide insight into policies to improve equity in asymmetric games.

Games played on asymmetric networks are one important class and can naturally become a source of asymmetry between players. Specifically, the asymmetric network governs the interactions among players such that only a few neighbors are capable of influencing a given player's set of decisions [28]. If this influence is biased in one direction, then the network position of certain players may be advantageous in space, time or both. Players with these positional advantages could be indifferent to or even exploit the strategies of others and thereby create an asymmetric game. Stackelberg games are an important example of the latter. The difference is that in Stackelberg and leader-follower games more generally, e.g., mathematical program with equilibrium constraints (MPECs) or equilibrium problems with equilibrium constraints (EPECs) [21], the leaders directly take into account the actions of the followers in their decision-making to optimize their own objective functions. The followers are passive and take the leaders' decisions as given.

The study of asymmetric games in this chapter concentrates on an asymmetric network that takes inspiration from river systems with multiple independent water users. Specifically, the players located on the upstream end of the river have a positional advantage manifesting as privileged access to water. Downstream users must take these decisions as given, which may result in excess flooding, inadequate water supply, or degraded water quality. Independent, conflicting water usage decisions often arise in trans-boundary river basins. Namely, these include situations where the river basin is not solely contained within one administrative boundary. This general situation is known as the river-sharing problem [29].

With this example in mind, this chapter considers a general, asymmetric game on a line-graph network where a shared resource is accessed on a first-come, first-served basis. In such a network, each player is sequentially positioned in a line on a directed network [29]. Excluding the two terminal-end players, each player has both an upstream and downstream neighbor. The two terminal-end players have only one upstream or downstream neighbor depending on the position. The upstream users are like leaders in a Stackelberg game, except they may not directly exploit the downstream users (e.g., are indifferent to followers). In the sections that follow, truly indifferent leaders are modeled equivalently as those who are abstaining from exploiting the followers.

Using this general model, this chapter provides several non-cooperative game theory models for linear-graph networks of river systems. The aim is to allow the downstream players to balance this asymmetry through payments to water-release markets. Compared to other papers in this line of research, the non-cooperative approach provides more realistic modeling as compared to cooperative game theoretic ones [30] yet still allows for an improved system benefit as compared to the current one. There are a number of important examples of these asymmetric games in a variety of different areas. Similarities and differences between river basins and other infrastructure systems are discussed in the next section.

2.1.2 Water vs. Other Infrastructure Systems

Water resource-related risks are closely linked to a number of ongoing economic and environmental concerns and have been exacerbated in recent years. The myriad causes include rapid population growth and urbanization, increased wastewater discharges and more stringent effluent limits, a greater number of recreational users, degraded in-stream environmental habitats and landscapes, increased frequency and duration of extreme weather events, and inequitable access to clean drinking water. For instance, the current drought in the Western United States is the worst in 1,200 years [31]. Stakeholders are recognizing that the future is rapidly coming into focus: tackling complex challenges requires a unified collaborative approach and cutting-edge solutions to evaluate and mitigate future risks. Furthermore, translating the flow of water into the flow of benefits is inherently challenging because of water's ubiquitous usage across municipal, agricultural, and industrial sectors. This hinders the ability to validate and address the associated inequities with regulation alone.

What makes water management and river systems in particular interesting and the focus of the application in this chapter, is their relationship to commodity markets. In general, there are no widely-implemented market structures to balance the asymmetry outlined above either for water quantity or quality. For example, the doctrine of prior appropriation in the western United States grants water rights on a first in time, first in right basis [32]. However, this system is rigid and does little more than transfer a spatial asymmetry into a temporal asymmetry. In contrast, other infrastructure systems can have market structures/systems to balance welfare and other system-level economic or other objectives. The examples that follow highlight this point.

In the electric power sector, markets in Europe and North America have several stages of decisions leading up to real time. For example, power producers can submit day-ahead bids for production levels and prices which then help independent system operators (ISOs) to balance power supply with forecasted demand. There are also markets that balance supply and demand in near real-time or automatic adjustment in real-time as well e.g., PJM power market in the U.S. (https://www.pjm.com/ or Nordpool in Europe (https://www.nordpoolgroup.com/).

Relative to water volumes, water resources don't operate with these levels of decision-making in part because they can store water as needed. In power systems, in today's markets there are generally no market-scale storage assets to mitigate potential imbalances in uncertain supply (i.e., renewable) or uncertain demand. Also, power markets allow for forward contracts as well as spot markets to be as flexible as possible, which is distinct from river-based water systems. One aspect that is akin to balancing upstream and downstream players in power is what is called demand response. This is temporal shifting of the consumer load (e.g., residential, industrial) to better balance supply and demand. For example, the residents in buildings may be incentivized with payments to shift their load to hours with lower prices for overall system benefit (i.e., less need for expensive and fossil fuel-based peaking plants). In this sense, the asymmetric game is over time with the upstream players the consumers (or producers) that are paid to alter their consumption (production) schedules for temporally later consumers or producers (i.e., downstream players) [33]

In transportation, specifically traffic management, there are also mechanisms in place to better balance the asymmetry in this transport infrastructure on a real-time basis. Consider real-time tolls that change their prices based on the volume of flow along a particular highway through the use of vehicle transponders. In effect, drivers can decide to use the roads later if the prices are too high. The earlier drivers in this case are the upstream players whose choice of using the tolled road can affect later, downstream drivers. In this case the asymmetry is over time but the earlier drivers are negatively incentivized by much higher congestion tolls (assuming that they are driving during the busy hours) [34].

From a water-quality perspective, the analogy with power is perhaps best through carbon emissions-reduction programs like the U.S. Regional Greenhouse Gas Initiative (RGGI) [35]. This program gives certain carbon allowances (maximum amount of tons of carbon emissions), and it's up to the market to identify cost-efficient emission reductions that satisfy these allowances. For example, power companies that produce renewable energy or can limit their carbon emissions can generate revenue from selling their unused allowances. Power companies that produce too much carbon emissions have to pay for this overage. It seems that RGGI has done well to monetize carbon emissions reductions. From this perspective, RGGI relates to water quality for example, sediment or pollution reduction in river systems. While power has such systems and markets in place, it is rarer for water systems to apply them successfully. The Virginia Nutrient Credit exchange program is a notable exception [36]. Another interesting comparison between water and power is that in water systems water users along a river can act as both suppliers and consumers, which is analogous to prosumers in energy markets.

2.2 Literature Review and Contributions of This Chapter

2.2.1 Literature Review

Most if not all of the research on line-graph games has been from the framework of cooperative game theory. Brink et al. (2007) used cooperative game theory to analyze line-graph games with applications in machine sequencing games and the river-sharing problem [29]. Khmelnitskaya (2010) extended this work to a more general case, which considers cooperative game theory on rooted-tree and sink-tree digraphs [37]. This structure was then used to address the river-sharing problem for more complex networks. These works demonstrate that the river-sharing problem can be generalized to a mathematically abstract setting within a game-theoretic context.

Network games from the non-cooperative game theoretic framework have been researched, but lack coverage in line-graph games. For example, Cominetti et al. (2021) formulate the Buck Passing Game where the players attempt to pass a chore to other players in the network to minimize individual effort [38]. Zhou and Chen (2018) consider sequential consumption in networks during a firm's release of a new product [39]. It is similar to a line-graph game but involves more sophisticated network dynamics. Parise and Ozdaglar (2019) formulate a general, variational inequality framework for network games, but do not cover line-graph games as a specific case [28].

Water-resource problems have been analyzed from a wide variety of both cooperative and non-cooperative game theoretic network contexts. Dinar and Hogarth (2015) presented a systematic review of game theory and water resource literature [11]. They found that much of this research was related to cooperative game theory. They also found that the non-cooperative models lack extensive formulations from an equilibrium programming perspective. Bekchanov et al. (2017) reviewed over 150 papers on water economic models. They concluded that the literature poorly integrates economic equilibrium models with the underlying water resource networks [12]. Archibald and Marshall (2018) corroborate this viewpoint in their literature review. They reviewed nearly 450 papers on mathematical programming in water resources, but equilibrium programming was notably absent [9].

Britz et al. (2013) provide a notable exception to the equilibrium programming gap in the literature. They model a stylized river basin using multiple optimization problems with equilibrium constraints [14]. In a follow-up paper, Kuhn et al. (2014) extend the approach to a real-world case study in Kenya's Lake Naivasha Basin. Despite the uniqueness of the approach, both of these papers do not attempt to generalize it to the general non-cooperative game theoretic context. They also focus primarily on water allocation issues without considering the trade-offs between water use curtailments and water infrastructure investment. Additionally, they do not consider nuances of water balances such as the role of indirect water reuse.

2.2.2 Contributions of the Current Chapter

This chapter formalizes the modeling approach used in [14] as a Generalized Nash equilibrium model for asymmetric, non-cooperative games on line graphs. It also provides a counterpoint to the cooperative game theory approach that is already well covered in the literature. The goal is to demonstrate how self-enforcing agreements are possible among players even in the context of an asymmetric game. Specifically, market structures are used to identify trading opportunities that connect high marginal benefits downstream to lower marginal costs upstream. It also considers water management decisions beyond water allocation such as the role of consumptive use, indirect water reuse, storage, and capital projects.

Furthermore, the proposed water release market is more tangible than markets based on water allocation. In the water release market, water's scarcity and associated value are based on the physical barriers and cost of releasing additional water to the river. In contrast, water-allocation markets are based on legally increasing a water-withdrawal limitation. Thus, the value of water is derived from scarcity associated with a legal barrier. In countries such as Chile, real-world implementation of these water-allocation markets are inequitable because the judicial system has not uniformly enforced this legal barrier [40].

To illustrate the approach, the model is applied to a stylized river basin as well as a case study in the Duck River basin in Tennessee, USA. This chapter considers the role of consumptive use, indirect water reuse, storage, and capital projects in water resource systems. The purpose is to extend the application of the approach used in [14]. Taken together, the application goal is to develop a collaborative approach to water resources management to better balance the upstream-downstream asymmetries. This chapter achieves this goal using concepts from other infrastructure markets and economic theory.

Summarizing the above discussion, the current chapter makes valuable contributions as follows: 1. Formalize non-cooperative games on line graphs as a counterpoint to the existing cooperative game theory literature; 2. Extend non-cooperative river basin game theory models to consider engineering-economic decisions beyond water allocation schemes, and 3. Create novel water market structures to achieve a better alignment of stakeholder interests in a river basin.

2.3 General Model

2.3.1 Line-Graph Network Games

The line-graph network game is a sequential game of $|I|$ turns, in which player $i \in I$ derives a payoff from depleting a shared resource down to a level s_i. This process repeats for player $i+1, i+2, ...$ until the final player $|I|$ takes their turn. Player i's payoff is dependent on the state, S, of the shared resource, which is represented as the depletion level inherited from the previous player: $S = s_{i-1}$. This paradigm could apply to games with first-come, first-served access (e.g., queuing problems) or to games with directed network flows (e.g., river basins or supply chains).

Sequential optimization models are used to represent the line-graph game mathematically in which $S \in \{s_o, s_1, s_2, ..., s_{|I-1|}\}$ is a dynamic parameter linking the models. The initial value s_o represents the starting state of the resource prior to the game. Additionally, let $x_i \in R_i(S) \subseteq \Re^n$ denote player i's n decisions that are possible given a resource state S. This chapter assumes for simplicity of notation that each player faces the same number of decisions. Furthermore, let $f_i^{LG}(x_i) : \Re^n \rightarrow \Re$ denote the associated payoff function and let the function $g^{LG}(x_i; S) : \Re^n \rightarrow \Re$ describe the relationship between player i's decisions, x_i, and the resulting depletion level s_i. This game can be expressed in algorithmic form as follows:

For each $i \in I$:

1. *if i = 1:* $S = s_o$; *else*: $S = s_{i-1}$

2. *Solve* $\max_{x_i} f_i^{LG}(x_i) \quad s.t. \quad x_i \in R_i(S)$

3. $s_i = g^{LG}(x_i^*; S)$

4. $i = i + 1$

This formulation illustrates how players at a positional disadvantage (i.e., late in the sequence) inherit the shared resource. They are completely dependent on the optimal decisions, x_i^* of the players early in the sequence yet have no direct opportunity to influence them. For future reference, the model described in Section 2.4.4.3 can be solved using this algorithm. The model represents the a river basin as a line graph with players ordered from upstream to downstream, and the dynamic parameter S equals the minimum water outflow ($O_{i-1,t}^{min}$), which is introduced in Section 2.4.2.

2.3.2 Generalized Nash Reformulation

The line-graph network structure does not preclude the players from other types of interactions such as allocating the shared resource in a market. This problem is now reformulated to allow these interactions to reduce the asymmetric resource access. The sequential algorithm no longer applies because market interactions are typically simultaneous. Consequently, the depletion levels, s_i, can be directly incorporated into the model without the sequential updating of S. The models presented in Sections 2.4.4.1 and 2.4.4.2 are examples of this reformulation. These models also represent the river basin as a line graph but have market interactions in the form of water sales flowing downstream to water purchasers.

In general, this reformulation is expressed in the form of (2.1) where each player simultaneously solves the following optimization problem:

$$max_{x_i,y_i,z_i} f_i^{GN}(x_i, y_i, z_i, \pi) \tag{2.1a}$$

$$\texttt{s.t.}$$

$$x_i, y_i, z_i \in R_i^{GN}(s_{i-1}) \tag{2.1b}$$

The vector $x_i \in \Re^{n_x}$ has the same definition as described in the previous section. The vector $y_i \in \Re^{n_y}$ represents player i's decisions that desirably influence players with better resource access to alter their depletion of the shared resource. An example of this is water purchases, $W_{i,t}^P$, which are introduced in Section 2.4.2. Conversely, the vector $z_i \in \Re^{n_z}$ represents player i's accommodations for players with worse resource access. An example is the water-loss reductions, $L_{i,c,t}^R$, which are also introduced in Section 2.4.2. The variable $\pi \in \Re^{n_\pi}$ is a vector of variables unique to the system that informs each player's decisions (e.g., market prices).

This is a generalized Nash problem because the constraint region, R_i^{GN}, is affected by other players' decisions, which is captured in the following mathematical expressions:

$$s_i = g^{GN}(z_i; s_{i-1}), \pi = h(Y, Z) \tag{2.2}$$

The function $g^{GN} : \Re^{n_z} \to \Re$ describes the value for the depletion level s_i on the domain of player i's feasible accommodation decisions, z_i, and the feasible states of the inherited resource, s_{i-1}. In the simplest form, this function could include conservation of flow constraints. In its most complex form, this function could include resource depletion estimates from a physical simulation. The function h transforms the vector of decisions $Y = (y_1^T, ..., y_{|I|}^T)^T$ and $Z = (z_1^T, ..., z_{|I|}^T)^T$ to some system value π (e.g., market price).

Generalized Nash problems are special cases of quasi-variational inequality problems which are more computationally challenging to solve than Nash games. In the latter case, just the objective functions of the various players show interactions with the decision variables of the other players. For generalized Nash problems, each player's constraint set can also be changed by the other players' decision variables, which is a more complicated situation but consistent with some shared resources. However, it is well-known that if the Lagrange multipliers to any shared constraints have the same value for each player (e.g., same value of the resource), then there is an equivalent variational inequality problem (or mixed complementarity problem) which is easier to solve [41], [42]. For recent references, see also [43] and [44] for a more general treatment of generalized Nash games. The former reference discusses generalized Nash games on networks and the latter considers a more general setting.

2.3.3 Cooperative Game Theoretic Considerations

Concepts from cooperative game theory are used to compare alternative systems or rules for specific implementations of the Generalized Nash Reformulation. These include the concepts of the coalition, the characteristic function, and the imputation. In this section, each concept is introduced in general and then adjusted to fit the context of the chapter.

A coalition represents a subset of players $I^C \subseteq I$ cooperating towards a common goal. One typically analyzes many distinct I^C to obtain a particular solution concept (e.g., core, Shapley values). However, in the context of (2.1) and (2.2), it is assumed that an equilibrium from a mathematical program can serve as a solution concept under certain conditions. Accordingly, this chapter considers I^C that are associated with an equilibrium solution:

$$I^C = \{i| \quad ||y_i|| \neq 0\} \cup \{i| \quad ||z_i|| \neq 0\} \tag{2.3}$$

where y_i and z_i are the same variables defined previously and $||\cdot||$ is any vector norm.

The characteristic function $v(I^C)$ gives the payoff that the members of I^C are guaranteed to receive if they act together as a coalition [45]. One typically analyzes a single game and thus expresses the payoff in absolute terms. However, in this context, the payoff is expressed as the surplus of the Generalized Nash Reformulation over the Line Graph Game:

$$v(I^C) = \sum_{i \in I^C} \left(f_i^{GN}(x_i^*, y_i^*, z_i^*, \pi) - f_i^{LG}(x_i^*) \right) \tag{2.4}$$

where x_i^*, y_i^*, z_i^* represent optimal decisions for player i. This definition was chosen because the line graph game represents the default situation of the players. In contrast, the Generalized Nash Reformulation represents the improvement from cooperation.

An imputation is defined mathematically as follows [45]:

$$v(I) = \sum_{i=1}^{|I|} r_i, \tag{2.5a}$$

$$r_i \geq v(\{i\}) \quad \forall i \in I \tag{2.5b}$$

where r_i is the reward player i receives from participating in the coalition. The first condition states that the rewards distributed to all players must equal the value of the characteristic function composed of all players. The second condition states that participating in the coalition should not decrease the rewards received. Put another way, joining the coalition of the group should provide a higher reward than the coalition of only oneself. Therefore, an imputation must maximize the payoff to the coalition and leave no player worse off than they would be independently. It effectively is a condition for mutual interest among the participating players.

Theorem 1. *A non-negative reward r_i for all players is a sufficient condition for an imputation in this optimization-based, line-graph game.*

See Appendix A.1 for the proof. Using these metrics, the solutions of alternative reformulations shown below are compared and contrasted using the associated characteristic functions and the criteria for imputations. Specifically, this chapter seeks alternative reformulations with high characteristic function values that are also imputations. Such conditions represent interactions that are non-cooperative fundamentally but are mutually beneficial for the players.

2.4 River Basin Equilibrium Model Formulations

This section presents a special case of the general line-graph model applied to water resources in river basins. Two alternative Generalized Nash reformulations are considered in Subsections 2.4.4.1 and 2.4.4.2. In both cases, the interaction structure between the players (i.e., the π function in (2.2)) is a water-release market. Subsection 2.4.4.3 considers the original line-graph game without any market to allow interaction between the players. Finally, Subsection 2.4.5 translates the cooperative game theory concepts into performance metrics for the market structures.

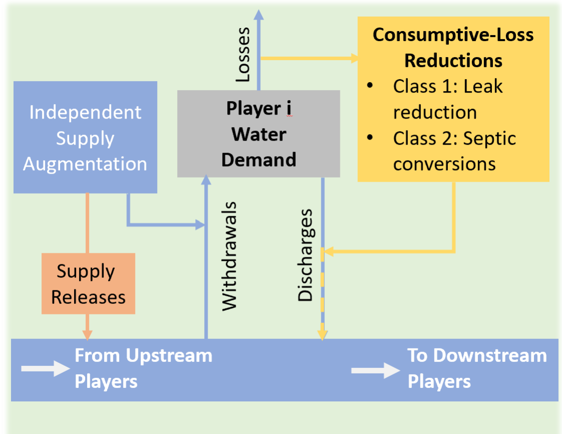


Figure 2.1: Hydrology and flow balance in the river basin for player i

2.4.1 Model Overview

Figure 2.1 depicts the flow balance for a particular river user, referred to as player i. The water available to player i is a function of the flow rate in the river as well as water released from upstream players. Player i can withdraw river water from an intake and combine it with an independent water supply, which typically represents a capital project such as a reservoir or pumped groundwater. The total water withdrawn is used to meet demand. A fraction of this water usage is returned to the river as discharges in the form of runoff, wastewater, or both. It recombines with the river water and flows to downstream players. The remaining water fraction is returned to the groundwater or another basin. This fraction is called consumptive losses because they effectively are unavailable for downstream players.

Releases from independent water supply infrastructure are one mechanism to increase reliable flows in the river. Specifically, water is released from a structure, such as a dam, into the river to increase the consistency of water flow. It typically provides a significant effective capacity increase over the natural flows in the river. A player in control of such infrastructure often gains a level of independence from other players. Thus, modeling infrastructure of this type extends beyond water allocation schemes because supply can often be increased if demand is high enough.

Reductions of consumptive losses are another mechanism to increase flows in the river. These reductions involve alterations such that more water is returned to the river as wastewater or runoff. One of the largest classes of consumptive losses is aging infrastructure. In this case, leaks from water mains or sewers enter the groundwater. Repairing the infrastructure reduces these losses from the river. Another class of losses are septic systems in rural and suburban areas, which return treated wastewater to the groundwater. Converting septic systems to sewers increases the return flow to the river via central wastewater collection and treatment.

The cost profiles associated with these two sources of water releases are nearly opposite. The capacity of the independent supply infrastructure is considered to be fixed, which reflects the large fixed costs of water supply infrastructure. However, the marginal costs are low and the potential releases are high. By contrast, consumptive-loss reductions are much more diffuse. For instance, many water mains would likely need to be repaired to generate a significant increase in return flows. Accordingly, the capacity of the consumptive-loss reductions are modeled as a continuous variable. To model diminishing returns, the marginal costs are considered to be progressively higher as more consumptive-loss reductions are implemented.

Having considered a single player, one can envision a market structure connecting the decisions of multiple players together. Figure 2.2 depicts the high-level function of the proposed water-release market. Downstream players (e.g., Player 2) purchase water from this market, which is supplied by upstream players (e.g., Player 1). This supply takes the form of water releases from independent supply sources and consumptive-loss reductions. The market prices

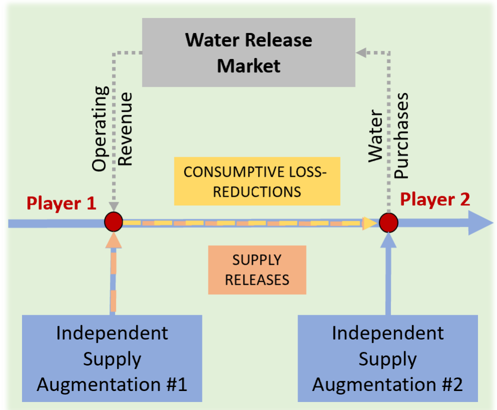


Figure 2.2: High-level view, water-release market (just 2 players) shown

cover the cost of these releases and could also provide additional revenue to incentivize upstream players to participate.

2.4.2 Notation

The notation in the model consists broadly of sets, primal variables, dual variables, and parameters. In the formulation, these are either units of flow or unit costs per flow rate. In the results section, flow rates are expressed in million gallons per day (MGD), or equivalently, thousand cubic meters per day (TCMD). Notation representing unit costs are expressed in discounted million dollars/MGD/planning period ($\$M/MGD$), or equivalently, discounted million dollars/TCMD/planning period. ($\$M/TCMD$). These latter units were chosen to represent flow rates conventionally while allowing total costs to be calculated over longer planning periods.

Sets

The sets in the model are listed below. Aliases are provided to allow the calculation of cumulative values arising from the use of these sets in the model. The brackets are omitted when referring to the cardinality of these sets.

- $i, j, k \in I$ = indexed users of the river from upstream to downstream
- $U_i \subset I$ = upstream nodes of i, where $j \in U_i$ is a typical node index
- $D_i \subset I$ = downstream nodes of i, where $k \in D_i$ is a typical node index
- $c \in C$ = classes of water loss reductions in ascending order of expense
- $t, t' \in T$ = budgetary planning time periods

Primal Variables

The following consists of the primal variables in each user's optimization problem. In this context, reliable capacity is a deterministic equivalent corresponding to a reasonable probability that the supply will be available to meet water demands. These variables represent steady state flow rates that occur during a much longer time horizon (i.e., planning period t).

- $W^D_{i,t}$ = player i's incremental increase in direct water withdrawal from the river relative to time period t-1 (volume/day)
- $W^S_{i,t}$ = player i's water supply sources from capital improvements that are independent of upstream releases (volume/day).
- $Q_{i,t}$ = player i's total demand in time period t (volume/day)
- $K_{i,t}$ = player i's reliable capacity added from capital project in time period t (volume/day)
- $L^R_{i,c,t}$ = player i's incremental water loss reductions in class c in time period t (volume/day)

- $W_{i,t}^{P}$ = player i's water purchases from upstream in the cost-sharing market formulation to reduce asymmetric access to water in time period t (volume/day)
- $W_{i,j,t}^{P}$ = player i's purchases from an upstream player j (volume/day)
- $W_{k,i,t}^{P}$ = water sales to player k downstream from i (volume/day)
- $O_{i,t}^{min}$ = player i's minimum water outflow to downstream nodes in time period t (volume/day)

Dual Variables

- $\gamma_{i,c,t}^{loss}$ = Nonnegative shadow price for loss reductions (cost/unit flow)
- $\gamma_{i,t}^{flow}$ = Nonnegative shadow price for withdrawal limitations (cost/unit flow)
- $\gamma_{i,t}^{cap}$ = Nonnegative shadow price for storage releases (cost/unit flow)
- $\lambda_{i,t}^{sup}$ = Unrestricted shadow price for total supply (cost/unit flow)
- $\lambda_{i,t}^{aug}$ = Unrestricted shadow price for supply augmentations (cost/unit flow)
- $\lambda_{i,t}^{rel}$ = Unrestricted shadow price for the minimum release downstream (cost/unit flow)
- $\pi_{i,t}^{as}$ = Nonnegative user i's price for reducing asymmetric access to water in time period t (cost/unit flow)

Functions

- $B_{i,t}$ = Concave consumer benefit function for player i at time t (currency)

- $R_{i,t}^{LR}$ = Revenue from loss reduction for player i at time t (currency)
- $V_{i,t}^{op}$ = Total operational costs for player i at time t (currency)
- $V_{i,t}^{inv}$ = Total investment costs for player i at time t (currency)
- $\theta_{i,t}(Q_{i,t})$ = Endogenously defined inverse demand curve as a function of total water demand $Q_{i,t}$ (cost/unit flow)

Parameters

- $c_{i,t}^{ops}$ = player i's unit operating costs in time period t (cost/unit flow)
- $c_{i,t}^{cap}$ = player i's unit capital construction costs in time period t (cost/unit flow)
- $c_{i,c,t}^{cu}$ = player i's unit cost for consumptive use reductions in class c during time period t (cost/unit flow)
- $c_{i,t}^{sr}$ = costs incurred per release of reliable storage capacity for player i during time period t (cost/unit flow)
- d_t = discount rate for time period t (%)
- $\delta_{ds_{k,i}}^{all} \in \{0, 1\}$ = logical parameter specifying if player k is downstream of player i
- $\delta_{us_{j,i}}^{all} \in \{0, 1\}$ = logical parameter specifying if player j is upstream of user i
- $lf_{i,c,t}$ = player i's estimated fraction of water losses in class c and time period t (%)
- n_i = local water inflow at player i independent of upstream players and capital improvements (volume/day)

- $r_{i,t}^{fc}$ = player i's regulator imposed flow constraint in time period t (volume/day)

- $a_{i,t}^{req}$ = player i's required augmentation for capital project in time period t that is varied to parameterize the equilibrium model (volume/day)

- $\alpha_{i,t}$ = inverse demand intercept for player i in time period t (cost/unit flow)

- $\beta_{i,t}$ = inverse demand linear slope for player i in time period t (cost/unit flow)

2.4.3 Formulation for Water Resource User $i \in I$

Each player represents a municipal water provider who is competing with other providers for access to water along a river. Specifically, each player must decide the values for the following set of variables, ζ:

$$\zeta = \left(W_{i,t}^{D}, W_{i,t}^{S}, Q_{i,t}, K_{i,t}, L_{i,c,t}^{R}, W_{i,t}^{P}\right)$$

The maximum payoff and constraints for player i's decisions are modeled as an optimization problem, which is represented as Program (2.6):

$$\max_{\zeta} \quad \left(\sum_{t=1}^{|T|} d_t(B_{i,t} + R_{i,t}^{LR} - V_{i,t}^{op} - V_{i,t}^{inv})\right) \tag{2.6a}$$

s.t.

$$\sum_{t'=1}^{t} L_{i,c,t'}^{R} \leq \sum_{t'=1}^{t} lf_{i,c,t'} W_{i,t'}^{D} \quad \forall c, t \quad (\gamma_{i,c,t}^{loss}) \tag{2.6b}$$

$$Q_{i,t} \leq n_i + W_{i,t}^{S} + W_{i,t}^{P} - r_{i,t}^{fc} + O_{i-1,t}^{min} \quad \forall t \quad (\gamma_{i,t}^{flow}) \tag{2.6c}$$

$$W_{i,t}^{S} \leq K_{i,t} \quad \forall t \quad (\gamma_{i,t}^{cap}) \tag{2.6d}$$

$$Q_{i,t} = \sum_{t'=1}^{t} W_{i,t'}^{D} \quad \forall t \quad (\lambda_{i,t}^{sup}) \tag{2.6e}$$

$$K_{i,t} = a_{i,t}^{req} \quad \forall t \quad (\lambda_{i,t}^{aug}) \tag{2.6f}$$

$$W_{i,t}^{D}, W_{i,t}^{S}, Q_{i,t}, K_{i,t}, W_{i,t}^{P} \geq 0 \quad \forall t, \quad L_{i,c,t}^{R} \geq 0 \quad \forall c, t \tag{2.6g}$$

(2.6a) represents the objective function for each player. It seeks to maximize social welfare. This is measured as the discounted consumer surplus of water use and the discounted revenue from the water release market less discounted capital and operating costs. The terms in each player's objective function are defined endogenously in terms of z and are described in Section 2.4.4.

(2.6b) - (2.6g) represent the constraints on each player's objective function. (2.6b) states that the loss reductions cannot exceed the losses from water withdrawals. (2.6c) states that the water withdrawn from the river is limited to the net inflow at a particular node minus the regulatory mandated stream flow. The net inflow depends on the minimum outflow from the player immediately upstream (i.e., player i-1). Thus, individual players can modify the constraint set of another player, which results in a generalized Nash equilibrium problem [42]. (2.6d) states that the water released from independent water supply sources must be less than or equal to the capacity of the associated capital project. (2.6e) states that the cumulative water demand consists of the sum of incremental direct water withdrawals up to the reference time period. Equation (2.6f) states that any capital project must be built in its entire capacity. The dual variables in parenthesis quantify how much each equation constrains the optimal objective function value.

2.4.4 Mixed Complementarity Problem Formulation

The water equilibrium model is formulated as a mixed complementarity problem (MCP). It consists of the concatenation of every player's Karush-Kuhn-Tucker (KKT) optimality conditions associated with (2.6), the endogenous functions listed in Section 2.4.2, and market-clearing conditions [21]. The KKT conditions are necessary because the constraints are linear. The sufficiency direction results since each player's optimization problem (2.6) is a concave maximization subject to polyhedral (hence convex) constraints.

The mixed complementarity problem generalizes the Karush-Kuhn-Tucker (KKT) optimality conditions of convex programs (with constraint qualifications), non-cooperative game theory, as well as a host of other problems in engineering and economics [21]. Formally, the MCP is defined for a given function F as finding $x \in R^{n_x}, y \in R^{n_y}$ such that

$$0 \leq F_x(x, y) \perp x \geq 0 \tag{2.7a}$$

$$0 = F_y(x, y), y \texttt{ free} \tag{2.7b}$$

where x is a non-negative vector and y is a vector of free variables. The particular form of the vector-valued function F is application-specific and below is described and related to mathematical optimization. The $\perp$ operator indicates that the product of the left and right sides of the expression must equal zero.

Two alternative water release market structures are considered within these assumptions: a general commodity market and a cost-sharing market. The asymmetric line-graph game without a market is also considered. These three structures result in different endogenous functions and market-clearing conditions. The similarities between them are described next, and their key features and differences are discussed in the subsections that follow.

Regardless of the market structure, there needs to be an expression defining the flow regime in the river that would result without any regulatory intervention or market. These are the flow conditions on which additional water purchases are based.

$$O_{i,t}^{min} = n_i - \sum_{c=1}^{|C|} \sum_{t'=1}^{t} lf_{i,c,t'} W_{i,t'}^{D} + \sum_{c=1}^{|C|} \sum_{t'=1}^{t-1} L_{i,c,t'}^{R} + O_{i-1,t}^{min} \quad \forall i, t \tag{2.8}$$

To serve this purpose, (2.8) establishes the minimum outflow conditions at each player's node. It is a function of the water withdrawal and release decisions and the minimum releases of the player immediately upstream (i.e., player i-1).

Both market structures share the same intrinsic consumer benefit function for player i's water withdrawals at time t. As shown in (2.9), it is represented as the area under a linearized water inverse demand curve θ with intercept $\alpha_{i,t}$ and slope $(-\beta_{i,t}) < 0$.

$$B_{i,t}(Q_{i,t}) = \int_0^{Q_{i,t}} \theta_{i,t}(x)\, dx = \int_0^{Q_{i,t}} (\alpha_{i,t} - \beta_{i,t} x\,) dx \tag{2.9}$$

$B_{i,t}(Q_{i,t})$ is concave since, by the Leibniz Integration Rule, $\frac{dB_{i,t}(Q_{i,t})}{dQ_{i,t}} = \alpha_{i,t} - \beta_{i,t} Q_{i,t}$ so that the second derivative is just $-\beta_{i,t} < 0$. Both market structures also share the same function for total investment costs. Thus the total capital investment costs for node i at time t is expressed as follows:

$$V_{i,t}^{inv}(K_{i,t}) = c_{i,t}^{cap} K_{i,t} \tag{2.10}$$

2.4.4.1 General Commodity Market (GCM) Formulation

In the general commodity market formulation (GCM), separate markets are established for each player generating water releases. Because of the market interactions, this model is an example of the Generalized Nash Reformulation described in Section 2.3.2. Downstream players submit bids to gain access to the water in each of these markets, and the water releases in each market are delivered to the downstream players with the highest willingness to pay at the market price. Intermediate players between the supplier and the purchaser are not allowed to use this water when it is released into the river system. This reflects the structure of general commodity markets where the supplier establishes a price, and the supply is divided among the various consumers purchasing goods at this price.

A key distinction between the market structures in the way water purchases are defined. For the general commodity market, water purchases are defined as follows:

$$W_{i,t}^{P} = \sum_{j=1}^{|I|} \delta_{us_{j,i}}^{all} W_{i,j,t}^{P} \quad \forall t \tag{2.11}$$

It states that the total water releases a recipient purchases is the sum of all the purchase requests to all upstream neighbors.

The revenue from water releases for node i at time t is defined in terms of the price at the supplying player's market:

$$R_{i,t}^{LR}(L_{i,c,t}^{R}, \forall c \in C) = \sum_{c=1}^{|C|} \pi_{i,t}^{as}(L_{i,c,t}^{R} + W_{i,t}^{S}) \quad \forall t \tag{2.12}$$

The total operating costs are defined in terms of the marginal costs of water conveyance and treatment, supply releases, loss reductions, and water purchase requests to upstream players:

$$V_{i,t}^{op}(Q_{i,t}, L_{i,c,t}^{R}, \forall c \in C, W_{i,t}^{S}, W_{i,j,t}^{P}, \forall j \in I, j \neq i) = \\ c_{i,t}^{ops} Q_{i,t} + \sum_{c=1}^{|C|} c_{i,c,t}^{cu} L_{i,c,t}^{R} + c_{i,t}^{sr} W_{i,t}^{S} + \sum_{j=1}^{|I|} \pi_{j,t}^{as} \delta_{us_{j,i}}^{all} W_{i,j,t}^{P} \quad \forall t \quad (2.13)$$

Loss reductions are considered incremental. Namely, loss reductions only need to be made in one time period because the measures to achieve them are usually permanent (e.g., water main leak reductions). Thus, the loss reductions only need to be paid for in one time period. In contrast, releases from independent water supply sources need to be purchased in each time period, because the measures to accomplish them are not permanent.

The market-clearing conditions say that the total amount of water demanded at node i by downstream nodes to balance asymmetry (left-hand side) should be less than or equal to what is made available by node i through loss-reduction efforts or releasing from independent water supply sources.

$$\sum_{k=1}^{|I|} \delta_{ds_{k,i}}^{all} W_{k,i,t}^{P} \leq \sum_{c \in C} L_{i,c,t}^{R} + W_{i,t}^{S} \perp \pi_{i,t} \geq 0, \forall t \quad (2.14)$$

Substituting these expressions into (2.6) yields the General Commodity Market (GCM) formulation for each player:

$$\max_{\zeta} \quad \sum_{t=1}^{|T|} d_t \Big(\int_0^{Q_{i,t}} (\alpha_{i,t} - \beta_{i,t} x) dx + \sum_{c=1}^{|C|} \pi_{i,t}^{as} (L_{i,c,t}^{R} + W_{i,t}^{S}) - (c_{i,t}^{ops} Q_{i,t} \\ + \sum_{c=1}^{|C|} c_{i,c,t}^{cu} L_{i,c,t}^{R} + c_{i,t}^{sr} W_{i,t}^{S} + \sum_{j=1}^{|I|} \pi_{j,t}^{as} \delta_{us_{j,i}}^{all} W_{i,j,t}^{P}) - c_{i,t}^{cap} K_{i,t} \Big) \quad (2.15a)$$

s.t.

$$\sum_{t'=1}^{t} L^{R}_{i,c,t'} \leq \sum_{t'=1}^{t} lf_{i,c,t'} W^{D}_{i,t'} \quad \forall c,t \quad (\gamma^{loss}_{i,c,t}) \tag{2.15b}$$

$$Q_{i,t} \leq n_i + W^{S}_{i,t} + \sum_{j=1}^{|I|} \delta^{all}_{us_{j,i}} W^{P}_{i,j,t} - r^{fc}_{i,t} + O^{min}_{i-1,t} \quad \forall t \quad (\gamma^{flow}_{i,t}) \tag{2.15c}$$

$$W^{S}_{i,t} \leq K_{i,t} \quad \forall t \quad (\gamma^{cap}_{i,t}) \tag{2.15d}$$

$$Q_{i,t} = \sum_{t'=1}^{t} W^{D}_{i,t'} \quad \forall t \quad (\lambda^{sup}_{i,t}) \tag{2.15e}$$

$$K_{i,t} = a^{req}_{i,t} \quad \forall t \quad (\lambda^{aug}_{i,t}) \tag{2.15f}$$

$$W^{D}_{i,t}, W^{S}_{i,t}, Q_{i,t}, K_{i,t}, W^{P}_{i,t} \geq 0 \quad \forall t, \quad L^{R}_{i,c,t} \geq 0 \quad \forall c,t \tag{2.15g}$$

As a reminder, the terms in parentheses next to each equation represent dual variables. The KKT conditions, endogenous functions, and market-clearing conditions are then concatenated to form a linear complementarity problem (LCP) as shown in Appendix A.5.

2.4.4.2 Cost-Sharing Market (CSM) Formulation

In the cost-sharing market (CSM) formulation, the restriction on intermediate players using water releases is relaxed. This allows multiple players to claim the same quantity of released water from an upstream player. While this is uncommon in most commodity markets, direct and indirect water reuse enables water supplies to be treated as a renewable resource. Indirect water reuse is common in river basins because treated wastewater discharges feed surface water intakes downstream [46]. Because of the market interactions, this model is also an example of the Generalized Nash Reformulation described in Section 2.3.2.

In contrast with the GCM structure, the markets are established at the purchasing player's node because water may be reused multiple times between the supplying and the purchasing player. Thus, the upstream players relative to the purchaser separately decide how much water releases to deliver based on the purchaser's willingness to pay. Conversely, the water release supplier receives revenue from all downstream users of this water. This market can be thought of as creating a mechanism for cost sharing through the rental of water.

In this structure, purchase agreements between players are no longer well defined. Therefore, water release purchases are simply the amount of water player i purchases. This makes the substitution of (2.11) into (2.6a) and (2.6c) unnecessary.

The revenue for node i's water releases at time t is similar to the GCM formulation, except the payment received for loss reductions is the sum of all the prices of the downstream players:

$$R^{LR}_{i,t}(L^R_{i,c,t}, \forall c \in C, W^S_{i,t}) = \sum_{k=1}^{|I|} \pi^{as}_{k,t}\delta^{all}_{ds_{k,i}}(\sum_{c=1}^{|C|} L^R_{i,c,t} + W^S_{i,t}) \quad \forall t \tag{2.16}$$

As before, the total operating costs are defined in terms of the marginal costs of water conveyance and treatment, supply releases, loss reductions, and water release purchases:

$$V^{op}_{i,t}(Q_{i,t}, L^R_{i,c,t}, \forall c \in C, W^S_{i,t}, W^P_{i,t}) = c^{ops}_{i,t}Q_{i,t} + \sum_{c=1}^{|C|} c^{cu}_{i,c,t}L^R_{i,c,t} + c^{sr}_{i,t}W^S_{i,t} + \pi^{as}_{i,t}W^P_{i,t} \quad \forall t \tag{2.17}$$

However, the cost for water releases is defined in terms of the price at the recipient player instead of the supplying players.

As in the traditional market formulation, loss reductions are permanent, and water releases from independent supply sources must be repurchased in subsequent time periods.

(2.18) represents the market-clearing conditions for player i's asymmetric access to water. It states that the losses reduced by the upstream players plus the amount released to the river from independent water supply sources place an upper bound on the purchases at node i. A positive price can only occur for these resources when the purchases equal the amount available upstream.

$$\sum_{i'=1}^{|I|} \delta^{all}_{us_{i',i}} (\sum_{c=1}^{|C|} L^R_{i,c',t} + W^S_{i',t}) - W^P_{i,t} \geq 0 \perp \pi^{as}_{i,t} \geq 0 \quad \forall t \tag{2.18}$$

Substituting these expressions into (2.6) yields the Cost Sharing Market (CSM) formulation for each player:

$$\max_{\zeta} \quad \sum_{t=1}^{|T|} d_t (\int_0^{Q_{i,t}} (\alpha_{i,t} - \beta_{i,t} x) dx + \sum_{k=1}^{|I|} \pi^{as}_{k,t} \delta^{all}_{ds_{k,i}} (\sum_{c=1}^{|C|} L^R_{i,c,t} + W^S_{i,t})$$
$$- (c^{ops}_{i,t} Q_{i,t} + \sum_{c=1}^{|C|} c^{cu}_{i,c,t} L^R_{i,c,t} + c^{sr}_{i,t} W^S_{i,t} + \pi^{as}_{i,t} W^P_{i,t}) - c^{cap}_{i,t} K_{i,t}) \tag{2.19a}$$

s.t.

$$\sum_{t'=1}^{t} L^R_{i,c,t'} \leq \sum_{t'=1}^{t} lf_{i,c,t'} W^D_{i,t'} \quad \forall c, t \quad (\gamma^{loss}_{i,c,t}) \tag{2.19b}$$

$$Q_{i,t} \leq n_i + W^S_{i,t} + W^P_{i,t} - r^{fc}_{i,t} + O^{min}_{i-1,t} \quad \forall t \quad (\gamma^{flow}_{i,t}) \tag{2.19c}$$

$$W^S_{i,t} \leq K_{i,t} \quad \forall t \quad (\gamma^{cap}_{i,t}) \tag{2.19d}$$

$$Q_{i,t} = \sum_{t'=1}^{t} W^D_{i,t'} \quad \forall t \quad (\lambda^{sup}_{i,t}) \tag{2.19e}$$

$$K_{i,t} = a^{req}_{i,t} \quad \forall t \quad (\lambda^{aug}_{i,t}) \tag{2.19f}$$

$$W^D_{i,t}, W^S_{i,t}, Q_{i,t}, K_{i,t}, W^P_{i,t} \geq 0 \quad \forall t, \quad L^R_{i,c,t} \geq 0 \quad \forall c,t \tag{2.19g}$$

The KKT conditions, endogenous functions, and market clearing conditions are then concatenated together to form this alternate LCP shown in Appendix A.6.

2.4.4.3 No-Market Formulation

This formulation represents no market-clearing conditions, as players only interact with each other through sequential water removal from the river. $L^R_{i,c,t}$ is equal to zero because there is no water release market to generate revenue. There is no incentive to reduce losses and no ability to make water purchases. Thus, this model is an example of the line-graph network game described in Section 2.3.1. The total operating costs are simplified accordingly:

$$V^{op}_{i,t}(Q_{i,t}, W^S_{i,t}) = c^{ops}_{i,t} Q_{i,t} + c^{sr}_{i,t} W^S_{i,t} \quad \forall t \tag{2.20}$$

Substituting these expressions into (2.6) yields the No-Market formulation for each player i:

$$\max_{\zeta} \quad \sum_{t=1}^{|T|} d_t \left(\int_0^{Q_{i,t}} (\alpha_{i,t} - \beta_{i,t} x) dx - (c^{ops}_{i,t} Q_{i,t} + c^{sr}_{i,t} W^S_{i,t}) - c^{cap}_{i,t} K_{i,t} \right) \tag{2.21a}$$

s.t.

$$Q_{i,t} \leq n_i + W^S_{i,t} - r^{fc}_{i,t} + O^{min}_{i-1,t} \quad \forall t \quad (\gamma^{flow}_{i,t}) \tag{2.21b}$$

$$W^S_{i,t} \leq K_{i,t} \quad \forall t \quad (\gamma^{cap}_{i,t}) \tag{2.21c}$$

$$Q_{i,t} = \sum_{t'=1}^{t} W^D_{i,t'} \quad \forall t \quad (\lambda^{sup}_{i,t}) \tag{2.21d}$$

$$K_{i,t} = a^{req}_{i,t} \quad \forall t \quad (\lambda^{aug}_{i,t}) \tag{2.21e}$$

$$W^D_{i,t}, W^S_{i,t}, Q_{i,t}, K_{i,t}, \geq 0 \quad \forall t \tag{2.21f}$$

Solving the No-Market formulation with an LCP is not necessary. It can be solved recursively using the algorithm presented in Section 2.3.1. However, the LCP Formulation is presented to be consistent with the other two Generalized Nash reformulations and is shown in Appendix A.7.

2.4.5 Performance Metrics

The cooperative game theoretic concepts described in Section 2.3.3 are used to create performance metrics for the GCM and CSM market structures. They are calculated from the optimal objective function values determined from the LCP solutions, which represent social welfare. The ultimate goal of the analysis is to test the effectiveness of each market structure in reducing the asymmetry between players.

The optimal objective function values are related to the rewards, r_i, that each player achieves. Let f_i^m represent the optimal objective function value for player i under market structure $m \in \{GSM, CSM\}$. These correspond to (2.15a) and (2.19a), which are both special cases of the generalized Nash reformulation objective function in (2.1a). Additionally, let f_{o_i} represent the optimal objective function value for player i in the no-market formulation. It is a special case of $f_i^{LG}(x_i)$ described in Section 2.3.1.

With these definitions in mind, the performance metrics from cooperative game theory can be expressed mathematically. The reward r_i^m each player experiences from participating in market structure m is the difference between the player's objective function value in market structure m and the no-market case:

$$r_i^m = f_i^m - f_{o_i} \tag{2.22}$$

Accordingly, the characteristic function for market structure m, $v^m(I)$, is simply the sum of the rewards across all players:

$$v^m(I) = \sum_{i \in I} r_i^m \tag{2.23}$$

The best performing market structures will be imputations and have large characteristic function definitions. With this in mind, consider a final metric representing the difference in characteristic function values between market structures m_1 and m_2:

$$v^{\Delta}(I) = |v^{m_1} - v^{m_2}| \tag{2.24}$$

In this particular case, m_1 is for the GCM market, and m_2 is for the CSM market. These metrics are used to analyze the numerical results presented in Section 2.5.

2.5 Results

This section discusses some theoretical results for the models proposed above with a focus on the GCM formulation for specificity. Additionally, sensitivity results are provided for a small stylized water system and numerical results for the Duck River in Tennessee, in the southeastern U.S. using real and realistic data to demonstrate insights of the models.

2.5.1 Theoretical Results

These theoretical results address existence and uniqueness of solutions as well as the relationships among important variables. As will be explained, the existence of solutions can be guaranteed in certain cases. In terms of uniqueness, there is the possibility for multiple solutions to the River Basin Equilibrium Model Formulation. An example with multiple solutions is provided in Section 2.5.2.1.

There are many variations in the water supply in solutions to the GCM model. For example, these variations could include more water from loss-reduction markets, water from extra supply based on capacity expansions, or decrease of demand. Accordingly, a simpler yet illustrative case of what could result is provided. The value of this illustrative case is the data input values that lead to one of these solutions in one case. It also illustrates the use of loss-reduction markets.

This representative case features just one time period $|T| = 1$, 1 loss-reduction class for each node, $|C| = 1$, and the optimization model that each node is trying to solve is adjusted accordingly. Note that there is now no discount factor (i.e., $d_t = 1$), L_i^R has no index for class nor time, and the incremental additions $W_{i,t}^D$ are now equal to Q_i so that equation from before relating them is now suppressed. Also, since the model is for the short term, there are no capacity decisions. Thus, $K_{i,t}$ and $W_{i,t}^S$ are no longer needed, nor are the associated dual variables to the corresponding constraints.

$$\max_{\zeta} \quad \int_0^{Q_i} (\alpha_i - \beta_i x)dx + \pi_i^{as} L_i^R - (c_i^{ops} Q_i + c_i^{cu} L_i^R + \sum_{j \in U_i} \pi_j^{as} W_{i,j}^P) \tag{2.25a}$$

s.t.

$$L_i^R \leq lf_i Q_i \quad (\gamma_i^{loss}) \tag{2.25b}$$

$$Q_i \leq n_i + \sum_{j \in U_i} W_{i,j}^P - r_i^{fc} + O_{i-1}^{min} \quad (\gamma_i^{flow}) \tag{2.25c}$$

$$Q_i, L_i^R, W_{i,j}^P, \forall j \in U_i \geq 0 \tag{2.25d}$$

In addition, the definitional and market-clearing constraints from before are suitably modified (i.e., the loss reductions happen and are used in the same time period):

$$O_i^{min} = n_i - lf_i Q_i + O_{i-1}^{min} \tag{2.26a}$$

$$\sum_{k \in D_i} W_{k,i}^P \leq L_i^R \perp \pi_i^{as} \geq 0 \tag{2.26b}$$

The next result is about existence of a solution for this one-period model (2.25) $\forall i \in I$ plus (2.26) and is presented below. For simplicity of illustration, it is assumed that there is just one upstream node u that delivers loss reductions, one downstream node d that receives it, and all other nodes e are inactive relative to the loss-reduction market. Clearly, other conditions on the data may lead to other solutions as this equilibrium problem has multiple solutions in general.

Theorem 2. *Consider the river system linear complementarity problem defined by the KKT conditions to (2.25) combined with (2.26) $\forall i \in I$. This problem always has a solution as long as the following conditions hold (assuming all positive cost coefficients):*

(i) $\beta_i > 0, \forall i \in I$

(ii) $c_e^{ops} - \alpha_e \geq 0$ *for all nodes e inactive in the loss-reduction market*

(iii) $lf_u Q_u = W^p_{d,u}$

(iv) $\sum_{r=1}^{e} n_r \geq r^{fc}_e$ *for all inactive nodes* e*.*

(v) $0 < \frac{\alpha_u - c^{ops}_u}{\beta_u} \leq \sum_{r=1}^{u} n_r - r^{fc}_u$ *for loss-reduction supplying node* u*.*

(vi) $c^{cu}_u \geq \alpha_d - c^{ops}_d$

(vii) $\sum_{r=1}^{d} n_r - r^{fc}_d = -\frac{\alpha_u - c^{ops}_u}{\beta_u} lf_u < 0$

where u, d, e *are respectively, the one loss-reduction market supplying node, the one loss-reduction receiving node, and any other node* e *not active in the loss-reduction market.*

See Appendix A.2 for the proof.

Note that in (i) $\beta_i > 0$ means that the demand function for each node i has a strictly decreasing slope which is quite reasonable. Also, the condition in (i) on the costs being nonnegative is also quite realistic. Condition (ii) amounts to saying that the operational costs for inactive node e exceed the highest demand α_e. Condition (iii) says that node $d \in D_u$ uses up 100% of the loss reductions from node u that is supplying it. Condition (iv) states that the inflows from upstream nodes are sufficient to cover the required flow constraints for each node e, which is inactive in the loss-reduction market. Condition (v) states that the extra supply at node u after accounting for inflows and flow constraints should be sufficiently large. Condition (vi) is a statement connecting the loss-reduction costs for upstream node u with the largest demand and operational costs for downstream node d. Lastly, (vii) states that the inflow to node d from all upstream nodes and itself less any flow restrictions should be sufficiently negative to induce water purchases from upstream node u.

The focus now returns to the original GCM model allowing for multiple time periods and loss-reduction classes. With this in mind, the next result concerns the prices at active nodes for the GCM model. Here the following notation is adopted: $U^+_{i,t}$ is the set of nodes upstream of node i where node i purchases loss-reduction measures at time t from node j, i.e., $U^+_{i,t} = \{j \in I : j \in U_i, W^P_{i,j,t} > 0\}$. Also, $D^+_{i,t}$ is the set of nodes downstream of node i where node i sells loss-reduction measures at time t to node k, i.e., $D^+_{i,t} = \{k \in D_i : W^P_{k,i,t} > 0\}$. The result below implies that the upstream loss-reduction markets must equilibrate in prices so that there is no arbitrage [1] opportunity among them relative to a fixed, downstream node i that wants these loss-reduction measures.

Theorem 3. *Consider node i in the GCM formulation and all upstream nodes $j \in U^+_{i,t}$. Then, $\pi^{as}_{j,t} = \pi_{i,t}, \forall j \in U^+_{i,t}$ where $\pi_{i,t}$ is a common loss-reduction market price for these nodes $j \in U_i$.*

See Appendix A.3 for the proof.

The next result is a statement about the uniqueness of the nodal prices for a fixed value of the dual variable $\gamma^{loss}_{i,c,t}$. This dual variable is associated with Constraint (2.15b) and it can be construed as the incremental value of one more unit of loss reductions. The first part of the next result (2.27a) states that the prices at a node i are the (discounted) sum of future values of $\gamma^{loss}_{i,c,t}$ plus the unit cost for consumptive use class c. This can be understood as the sum of the future opportunity costs plus the current operating cost of loss reductions. The second part of this result (2.27b) says that these nodal prices also are the discounted shadow price for downstream nodes $k \in D^+_{i,t}$ of getting one more unit of flow via the associated multiplier $\gamma^{flow}_{k,t}$ to constraint (2.15c). Thus, these nodal prices are computed to balance the economic needs of node i with its

[1] Arbitrage refers to the practice of buying a commodity in one market and reselling it for a higher price in another market.

downstream loss-reduction market customers.

Theorem 4. *Consider the GCM formulation and a node i for which there are loss reductions, i.e., $L^R_{i,c,t} > 0$ for some $c \in C, t \in T$. Then,*

$$\pi^{as}_{i,t} = \frac{\sum_{t'=t}^{|T|} \gamma^{loss}_{i,c,t}}{d_t} + c^{cu}_{i,c,t} \tag{2.27a}$$

$$\pi^{as}_{i,t} = \frac{\gamma^{flow}_{k,t}}{d_t}, \forall k \in D^+_{i,t} \tag{2.27b}$$

See proof in Appendix A.4.

Given that there are multiple solutions to the river basin equilibrium problem as indicated above, some other approach is needed to further refine the solution set. For example, one approach is to use equity-enforcing constraints or more generally logical constraints to filter out all but one solution as presented in the discretely constrained mixed complementarity problem (DC-MCP) formulations from [47, 48].

2.5.2 Numerical Results

2.5.2.1 Three-Node Model

A small but illustrative three-node model of the above two formulations was developed to illustrate the merits of the modeling approach and to compare the market structures. Three players, numbered sequentially in increasing order from upstream to downstream, represent producers, prosumers, and consumers of consumptive loss reductions, respectively. Two loss-reduction classes and two time periods give the model multi-dimensionality with respect to these parameters. To simplify the analysis, no capital projects are present.

The parameters for this system were chosen to represent a system with asymmetric access to water and intermediate water scarcity. Enough water is available in the first time period for two out of three players to completely satisfy their demand. In the second time period, the economic growth potential of all players is greater than the water available. To ensure asymmetry, all of the inflow into the river basin occurs at Player 1's node (n_1). Each player has the same regulatory flow constraint ($r_{i,t}^{f,c}$) representing the minimum base flow necessary to preserve the aquatic habitat. The overall intent is to fully utilize the market in time period 2 while illustrating reasonable starting conditions in time period 1.

Within these guidelines, various scenarios were developed to consider different types of river basins. Certain parameters were kept constant from scenario to scenario to keep them comparable. These include each player's operating costs ($c_{i,t}^{ops}$), the discount rate (d_t), and the inverse demand slope ($\beta_{i,t}$). The remaining parameters were varied across scenarios to ascertain the impact of different player configurations, supplies, and demands. These include the following four non-fixed parameters: the maximum demand in time period 1, the maximum demand in time period 2, the loss fractions ($lf_{i,c,t}$), and the consumptive use reduction costs ($c_{i,c,t}^{cu}$).

The demands were incorporated into the model via the inverse demand intercept ($\alpha_{i,t}$). Specifically, a point of known price and quantity was assumed to exist at the current demand level and operating cost ($c_{i,t}^{ops}$). Linearizing about this point for a given value of $\beta_{i,t}$ was then used to obtain the intercept value. (2.28) expresses this mathematically:

$$\alpha_{i,t} = \beta_{i,t} demand_{i,t} + c_{i,t}^{ops} \tag{2.28}$$

Table 2.1 summarizes the input data used in the three-node model scenarios. Each row

Table 2.1: Data used in the three-node model scenario analysis

Parameter	Player(s)	Time Period(s)	Class(es)	Value
int rate	1, 2, 3	1, 2		0.04
β	1, 2, 3	1, 2		3
n	1			9
	2, 3			0
rfc	1, 2, 3			4
c_ops	1, 2, 3			1
c_cu[2]	1, 2, 3		1	1
	1, 2, 3		2	5
demand[2]	1, 2, 3	1		5
	1, 2, 3	2		10
lf[2]	1, 2, 3	1, 2	1, 2	0.1

represents the unique value assigned to the parameter from the first column. The second, third, and fourth columns indicate the applicable indices for the given value assignment. For example, the inverse demand slope (β) is assigned a value of 3.0 for all three players in all three time periods. Consumptive loss-reduction costs, time period 1 demands, time period 2 demands, and loss factors are baseline values to be varied in the different scenarios [2].

The baseline values, which are the last three parameters in Table 2.1, are systematically varied among the players to investigate how player heterogeneity influences market structure. For a given scenario, the baseline values are each multiplied by a low (0.66), medium (1.0), or high (1.33) scaling factor to obtain the actual value of the parameter. To create this heterogeneity, no two players have the same scaling factor for a given parameter in a given scenario. Mathematically, this results in 3! = 6 ways to assign a player a value for a given parameter. For example, consider one of the six ways to assign the time period 2 demands among the players. The scaling

[2]For simplicity, only the baseline values themselves are depicted.

factors for players (1, 2, 3) are (medium, high, low) respectively such that the tuple of associated demand values is (10.00,13.33,6.66).

A given scenario consists of one of these player-specific tuples for each of the four baseline value parameters. Every combination of tuples for the four parameters were considered, which results in a sizable number of scenarios. Mathematically, applying the Cartesian product to the four non-fixed parameters results in $3!^4 = 1296$ scenarios total. Table 2.3 provides examples of final parameter values that correspond to scenarios analyzed closely in this section.

Each scenario was compiled and solved in GAMS [3] using an application programming interface with Python. Three separate models were solved for each scenario, which included the GCM, CSM, and no-market formulations. The solutions from these models were used to calculate the metrics detailed in Section 2.4.5. These are used to quantify the benefit of the GCM and CSM market structures relative to no market.

Table 2.2 summarizes the results of the various scenario runs in more detail. The first row depicts the percentage of the scenarios where the market structure in the corresponding column generated higher social welfare (i.e. $v^m(N)$) than the alternative (GCM or CSM). The second and third row depict the mean and standard deviation, respectively, of social welfare improvement as defined in Equation (2.6a). Lastly, the fourth and fifth rows depict the improvement of social welfare when the given market structure is higher-performing (i.e., $v^{\Delta}(N)$).

For every player in every scenario, at least one of the market structures improves social welfare compared to no market at all (i.e., $r_i \geq 0$). Therefore, the markets demonstrate mutual interest among the players (i.e., always form an imputation). However, not all the market structures result in mutually beneficial interactions. For instance, in some of the scenarios, the

[3] www.gams.com/

Table 2.2: Summary of scenario results

Metric	GCM	CSM
% higher $v^m(N)$	3.70%	96.30%
average $v^m(N)$	\$42.64	\$36.87
std. dev $v^m(N)$	\$0.74	\$11.96
average $v^\Delta(N)$	\$42.64	\$14.49
std. dev $v^\Delta(N)$	\$0.74	\$14.44

lower-performing market structure will not form an imputation. This illustrates why choosing the proper market structure is important.

For most of the scenarios, the CSM generates higher social welfare than the GCM. This occurs in over 96 % of the scenarios analyzed. However, the GCM vastly outperforms the CSM in this metric in the small number of its preferred scenarios. It reliably generates high social welfare improvements when it is the appropriate choice. The average and standard deviations for $v^m(N)$ and $v^\Delta(N)$ in Table 2.2 support this finding.

The furthest downstream player always undergoes dramatic economic growth for scenarios where the GCM has higher social welfare than the CSM. Specifically, Player 3 has a low demand in time period 1 and grows to have a high demand in time period 2. Under these conditions, Player 3 is most vulnerable to the decisions of Player 2. As will be explained, this vulnerability exists when the system-wide social welfare is most sensitive to the positional advantage of intermediate players along the network. This demand profile appears in all the cases where the GCM exceeds the CSM in social welfare.

The loss-reduction market, regardless of structure, is most effective relative to no market for a specific set of common scenarios. These occur when the time period 2 demands get progressively higher downstream and the losses get progressively higher upstream. This finding makes sense, because higher losses upstream lead to less water available downstream where it is most

Table 2.3: Parameter values used in the detailed analysis

Parameter	Scenario	Player		
		i = 1	i = 2	i = 3
$demand_{i,1}$	Large Prosumer	3.33	6.67	5.00
	D.S. Econ. Growth	5.00	6.67	3.33
	Multiple Prices	5.00	3.33	6.67
$demand_{i,2}$	Large Prosumer	6.67	13.33	10.00
	D.S. Econ. Growth	6.67	10.00	13.33
	Multiple Prices	10.00	13.33	6.67
$c_{i,1}^{cu}$	All Three	0.67	1.00	1.33
$c_{i,2}^{cu}$	All Three	3.33	5.00	6.67
$lf_{1,i,1}$	All Three	0.13	0.10	0.07
$lf_{1,i,2}$	All Three	0.13	0.10	0.07
$lf_{2,i,1}$	All Three	0.13	0.10	0.07
$lf_{2,i,2}$	All Three	0.13	0.10	0.07

valuable. Interestingly, these scenarios were relatively insensitive to the consumptive use costs. The demand and loss parameters seem to matter the most to the viability of the market.

With the aggregate results in mind, three scenarios were selected for detailed analysis. The objective was to identify a scenario for each market structure where the social welfare differences are the most pronounced. Mathematically, these are scenarios where $v^m(N)$ and $v^\Delta(N)$ are both high. The first scenario, hereafter called the Large Prosumer Scenario, was chosen to illustrate the merits of the CSM market. The second scenario, hereafter called the Downstream Economic Growth Scenario, was chosen to illustrate the merits of the GCM market. The parameter values used in these scenarios are shown in Table 2.3. This further reinforces the importance of the demand profile to the appropriate water-release market structure. Furthermore, a third scenario was selected to illustrate the non-uniqueness of prices as described in Section 2.5.1.

Figures 2.3a and 2.3b compare and contrast the market structures for the Large Prosumer Scenario, while Figures 2.4a and 2.4b do the same for the Downstream Economic Growth Scenario. All these figures depict the line graph of the river in plan view with the cooperative game theory metrics. Additionally, a profile view representing the flow levels in the river is depicted in millions of gallons per day (MGD). These plots have two key groups of elements warranting explanation.

The first group of elements includes the bars on the profile view. The stacked bar represents the actual inflow. It is subdivided into the freely-available inflow irrespective of the market structure plus additional inflow purchased from a market. The maximum usable inflow for each player is also plotted to gauge the level of scarcity of the actual inflow. In essence, it represents the inflow levels that the player would want to see in the river.

The second group of elements includes the line plots on the profile view. They represent how consumptive losses and the subsequent reductions impact the actual flows on the river. Specifically, the inflow without market represents the minimum river levels at a player's node if no consumptive-loss reductions were made. By contrast, the inflow with market represents the actual levels in the river including consumptive-loss reductions. If these two line plots are equal, then no consumptive-loss reductions were made. For additional clarity, Table 2.4 mathematically defines these elements and other terms used in the detailed analysis.

In the Large Prosumer Scenario, the CSM generates higher social welfare than the GCM because the former has higher resource utilization than the latter. In both market structures, Player 2 purchases inflow up to the amount made available through the markets. However, as shown in Figure 2.3a, Player 3's actual inflow in the GCM is less than the available inflow with the market. This difference between available and actual inflow used to meet demand represents

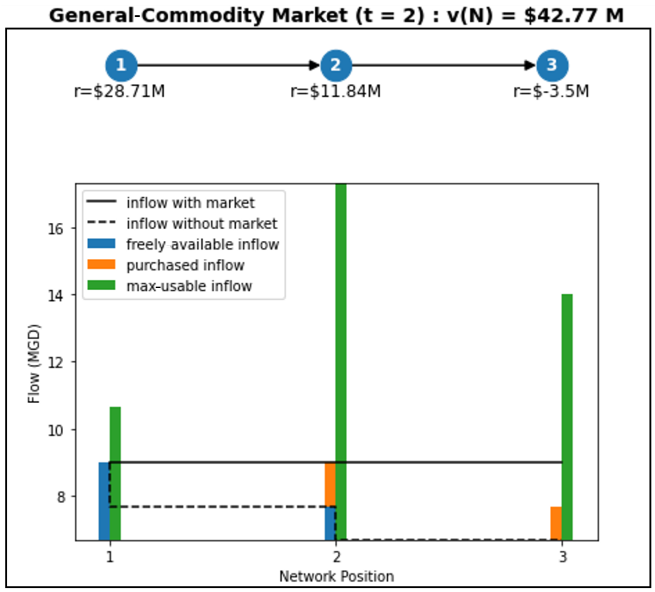
Table 2.4: Mathematical definitions for terms used in the detailed analysis

Term [Reference]	Mathematical Definition
inflow with market (MGD) [D1]	$n_i + O^{min}_{i-1,t} + \sum_{j=1}^{\lvert I \rvert} \sum_{c=1}^{\lvert C \rvert} \delta^{all}_{us_{j,i}} L^{R}_{i,c,t} + W^{S}_{j,t}$
inflow without market [D2]	$n_i + O^{min}_{i-1,t}$
freely available inflow (MGD) [D3]	$Q_{i,t} - W^{P}_{i,t} + r^{fc}_{i,t}$
max-usable inflow (MGD) [D4]	$demand_{i,t} + r^{fc}_{i,t}$
resource utilization (%) [D5]	$1 - \min\left\{ \frac{D1-(Q_{i,t}+r^{fc}_{i,t})}{D1}, \frac{D4-(Q_{i,t}+r^{fc}_{i,t})}{D4} \right\}$

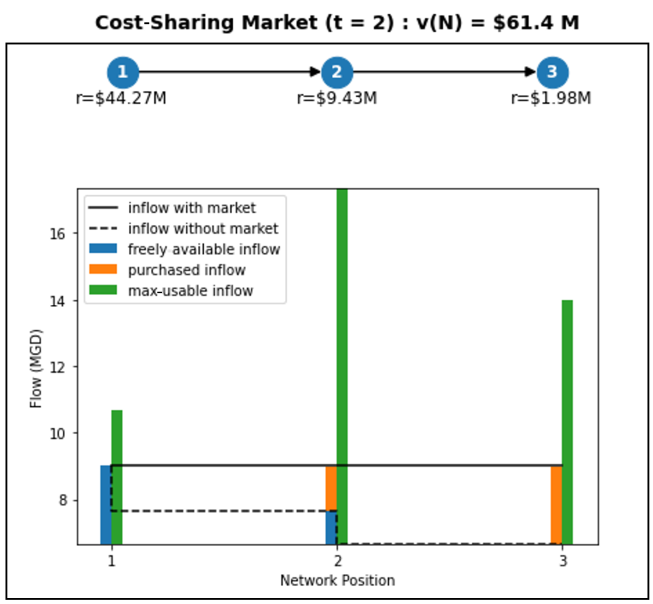
resource under-utilization because all the available inflow with the market is within Player 3's maximum usable inflow. By contrast, Figure 2.3b shows that both Player's 2 and 3 are able to purchase all the available inflow in the CSM.

The resource under-utilization in the GCM is a consequence of the structure of the market-clearing conditions. In (2.14), water-release purchases (i.e., $W^{P}_{k,i,t}$) are treated as bilateral agreements between a supplier i and a purchaser j. These agreements will increase the actual inflow in the river for all players downstream of Player i unless Player j's consumptive losses are 100%. However, the GCM structure only permits Player j to withdraw this added inflow. By contrast, the CSM relaxes the bilateral purchasing assumption (i.e., $W^{P}_{i,t}$) in (2.18) to allow multiple players to benefit from the water releases.

In the Downstream Economic Growth Scenario, the GCM generates higher social welfare than the CSM because the bilateral water purchases reduce the asymmetry in the network. As shown in Figure 2.4a, the GCM decreases the loss reductions that Player 3 needs to purchase (2.07 MGD instead of 2.33 MGD) to maximize social welfare. This occurs because the water Player 3 purchases from Player 1 is inaccessible to Player 2. In the CSM, no such restriction exists, so Player 2 uses this additional water as shown in Figure 2.4b. In doing so, Player 2 incurs



(a) General commodity market with resource under-utilization



(b) Cost sharing market

Figure 2.3: Visualization of the Large Prosumer Scenario. The cooperative game-theoretic rewards to each player, r_i^m, are shown in the plan view of the network. Water usage is shown in the profile view.

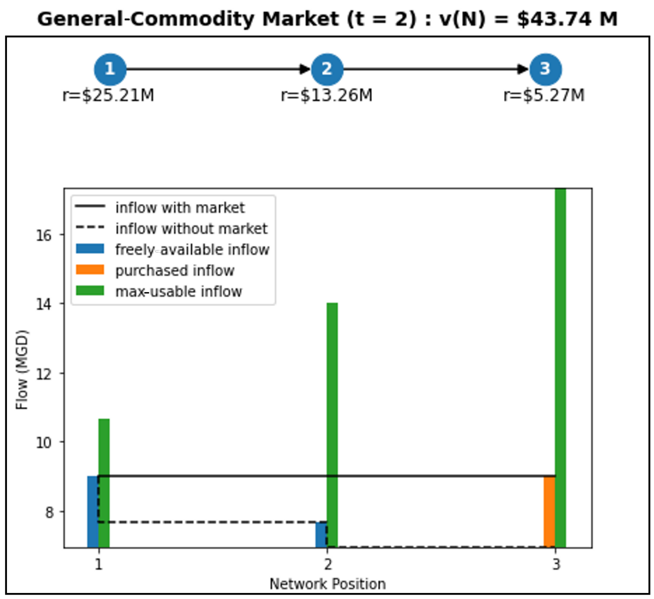
additional losses because it has a non-zero loss factor.

This scenario illustrates that the overall decrease in social welfare from intermediate losses can be significant because Player 2 values an incremental increase in consumption less than Player 3. Numerically, Player 3 has a higher γ^{flow} value than Player 2 (\$20.55 M vs. \$15.95 M, not depicted graphically), which represents the marginal value of additional water use. As alluded to earlier in this section, this phenomenon in the CSM market structure gives a positional advantage to intermediate players. Relative to the GCM, Player 2 increases water withdrawals and subsequently increases Player 3's consumptive loss-reduction purchases.

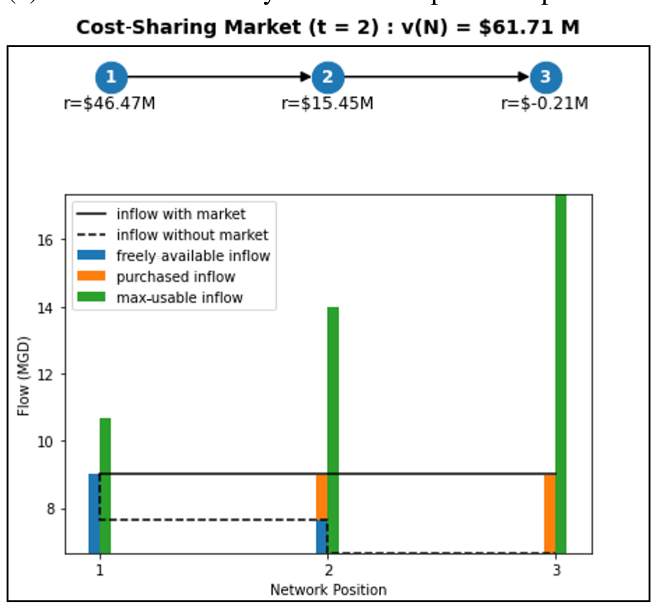
The Downstream Economic Growth Scenario also reveals an important nuance with regards to social welfare. The CSM model technically has a higher characteristic function value, but it is not an imputation because the reward to Player 3 is negative. Thus, the basin would not likely agree unanimously to implement this market structure. Alternatively, the GCM model is an imputation. Thus, the GCM is a more reasonable alternative for improving social welfare over the no-market structure.

In both scenarios, the figures for time period 1 were omitted because no purchases of loss reductions are made. This occurs because the players making loss reductions realize a higher price by waiting for demand increases. This can be observed mathematically in the stationary KKT conditions for loss reductions (Equations (A.3e) and (A.4e)). The tendency to withhold supply may offset some of the inherent advantages of market efficiencies.

Table 2.5 illustrates the non-unique solutions in the GCM market. The term V represents the starting point used for all the variables in the model. Thus, different solution starting points can be chosen to generate multiple solutions that satisfy Theorem 4. An equity-enforcing set of constraints found in discretely constrained MCPs would be one way to distinguish between



(a) General commodity market with purchase protection



(b) Cost-sharing market with intermediate positional advantage

Figure 2.4: Visualization of the Downstream Economic Growth Scenario. The cooperative game-theoretic rewards to each player, r_i^m, are shown in the plan view of the network. Water usage is shown in the profile view.

Table 2.5: Multiple Prices Scenario in the GCM market

Variable / Parameter	V = 2	V = 2000
$\gamma^{loss}_{2,1,1}$	0.71	1.34
$\gamma^{loss}_{2,1,2}$	6.84	6.52
$c^{cu}_{2,1,1}$	1	1
$\gamma^{loss}_{2,2,1}$	0	0.63
$\gamma^{loss}_{2,2,2}$	3.55	3.24
$c^{cu}_{2,2,1}$	5	5
$\sum_{t=1}^{2} \gamma^{loss}_{2,1,t} + c^{cu}_{2,1,1}$	8.55	8.87
$\sum_{t=1}^{2} \gamma^{loss}_{2,2,t} + c^{cu}_{2,2,1}$	8.55	8.87
$\pi^{as}_{2,1}$	8.55	8.87
$\gamma^{flow}_{3,1}$	8.55	8.87
$W^{P}_{3,2,1}$	0.67	0.68

multiple solutions [47, 48].

2.5.2.2 Duck River Model

Another model was generated for the Duck River in central Tennessee. This model was designed to evaluate the market approaches with real-world data and to explore the impact of capital projects. In the three-node model, no capital projects were considered. In contrast, the Duck River model seeks to understand how the water release market impacts the optimal timing of water infrastructure investments with large fixed costs. This use case is relevant to river basins in general because water scarcity usually serves as a driver for significant supply expansion. For context, a similar real-options approach was considered for a single-optimization problem in Chapter 18 of [46].

Stakeholders in the Duck River watershed have been navigating water resource-related challenges in earnest since the extreme drought of 2007. Seven water utilities in the Duck River watershed serve water to approximately 250,000 people and industries that include car manufacturers, food processing plants, and other businesses. In addition to these uses, the river provides a wide range of other values including recreation, an excellent fishery, and some of the most biologically-rich freshwater habitat in North America [49].

The drought of 2007 highlighted the issue that in extended dry weather conditions, the citizens of the Duck River region depend on the water stored in Normandy Reservoir to meet all designated uses, including drinking water, wastewater assimilation, recreation, and natural resource protection. The dramatic decrease in rainfall, combined with the multitude of uses of the reservoir and the river, caused record low water levels in Normandy Reservoir that resulted in temporary changes in dam operation to protect water uses. Weather patterns and growth projections, combined with the obligation to manage water resources responsibly for future generations, created the need for a comprehensive regional water supply plan for the Duck River Region. [49]

Development of the regional water supply plan [49] and a reservoir-river model of water budgets along the river highlighted the inequities in benefits between the upstream and downstream users in the basin [4]. Higher than normal releases from the reservoir to the river during extreme dry events resulted in impacts to the reservoir users due to excessive drawdown of the reservoir. In contrast, the flow constraint of 100 cubic feet per second (cfs) on just the most downstream user ignored consumptive water use by upstream water systems, golf courses, and other users.

While the river-reservoir model provided insights into water withdrawals and discharges along the river (i.e., water balance), improved decision-making tools are needed to gain a better understanding of the following questions:

[4]The OASIS software was used to build the reservoir-river model. More information can be found here: www.hazenandsawyer.com/publications/oasis-modeling-for-water-people/

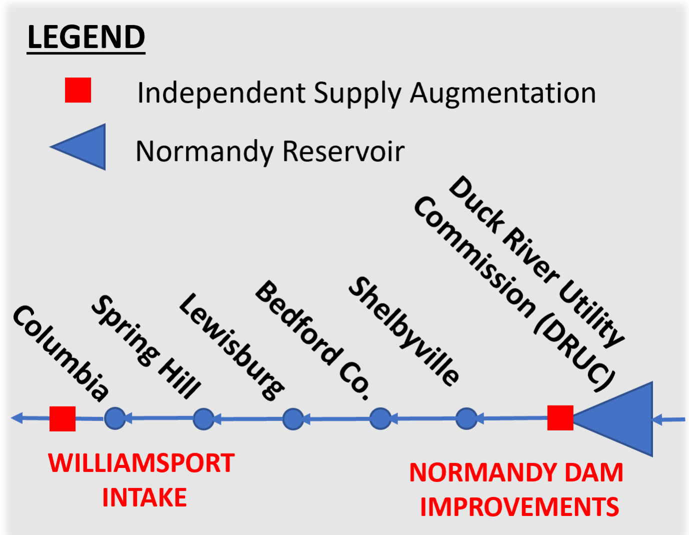


Figure 2.5: Schematic of the Duck River Agency's municipal users and relative positions along the river. Normandy reservoir is at the upstream end of the river. The flow direction is shown opposite of convention to reflect the east-to-west flow of the river.

- How does the flow of water in the Duck River translate into the flow of economic and environmental benefits for the individual stakeholders and the region?
- How can decision-makers overcome the strategic fragmentation that exists among stakeholders who individually may have an incomplete view of the "big-picture" problems for the region?
- How can water supply agreements and permits incorporate flexibility to overcome changing conditions?

Figure 2.5 depicts the line-graph network structure for the Duck River Basin. Contrasting with the previous example, there are six players considered instead of three. Each player is a municipal water provider for the named city or county with the exception of Duck River Utility Commission (DRUC). DRUC serves the cities of Manchester and Tullahoma using the water from Normandy reservoir at the upstream end of the basin. The Normandy dam separates DRUC from the rest of the downstream water providers.

Several data sources were consulted to estimate the model parameter values. The published water rates for each of the municipalities were used to estimate water operating costs. The water supply plan [49] and the drought management plan [50] were used to estimate water supply volumes, capital recovery costs, capital supply augmentation capacities, and regulatory flow constraints. Water demand projections and consumptive loss fractions were estimated from analysis associated with a demand projection study in the basin [51]. Industry-available data was used to estimate consumptive use costs and the inverse demand slope [52] [53] [54].

The primary water supply source for most of the basin is water released from Normandy reservoir. Historically, these releases have been at least 77.6 MGD at a 97 % reliability [5] [50]. Due to rapid growth in the region, water demands are expected to increase in the coming decades. Furthermore, consumptive use represents over a quarter of the water withdrawn from the basin in some cases [51]. Some users discharge wastewater outside the basin as well.

This supply and demand profile of the basin creates the potential for inequities in economic growth. Columbia is expected to grow from 7.54 to 12.74 MGD between the years 2015 and 2050. Despite the growth potential, Columbia has the least favorable access to water. First, it is the only water system with a regulatory flow constraint in its water withdrawal permit. The permit states that Columbia must cease all water withdrawals if the flow in the river decreases to 64.6 MGD. Additionally, it is the farthest downstream player, so the consumptive losses of upstream water systems can exacerbate Columbia's inequity.

The water supply plan for the Duck River Agency [49] identified two projects as alterna-

[5]This is based on the criteria for Stage 3 drought conditions, which represents the drought threshold necessitating the reduction of Normandy Dam outflows to 77.6 MGD. This condition is expected to occur once every thirty years.

tives to address this and other water supply related inequities in the basin. Figure 2.5 depicts the location of these proposed capital projects in the basin. The Normandy Dam improvements project would raise the Normandy dam to effectively increase the water stored in the Normandy Reservoir. Alternatively, the Williamsport project would create a new water intake at a less environmentally-sensitive location, which would allow for increased withdrawals from the river.

The latter alternative is incorporated into the present analysis because it has emerged as the higher-priority project for Columbia and the rest of the basin's stakeholders. The project enables Columbia to withdraw water without its regulatory flow constraint, which therefore improves its access to water significantly. It also decreases its dependence on releases from the Normandy reservoir, which leaves more water available for upstream players. Thus, the scenarios considered for this model involve the installation year for the Williamsport Intake project.

Assuming Columbia finances the project, the optimal timing for the investment is the key question underlying the scenario analysis in this model. Deferring investment is assumed to decrease project costs because long-term economic growth increases the available revenue for paying principal (instead of interest) on a loan. However, the decreased costs must be weighed against the benefits of the water supply increase. Furthermore, the role of the water release market must also be considered.

To answer this question, separate model runs for each market structure were performed for the installation years 2015,2020,..,2040,2045. It was assumed that Columbia bore the majority of the direct benefits and associated costs. Accordingly, the required augmentation parameter, $a^{req}_{columbia,t}$, and the capital cost parameter, $c^{cap}_{columbia,t}$, were manipulated from scenario to scenario. The former was set to the project's capacity, which is 64.6 MGD, for the installation year onward. The latter was set according to the simple formula: $c^{cap}_{columbia,t} = 5{*}[annual\_payment]/64.6$. This

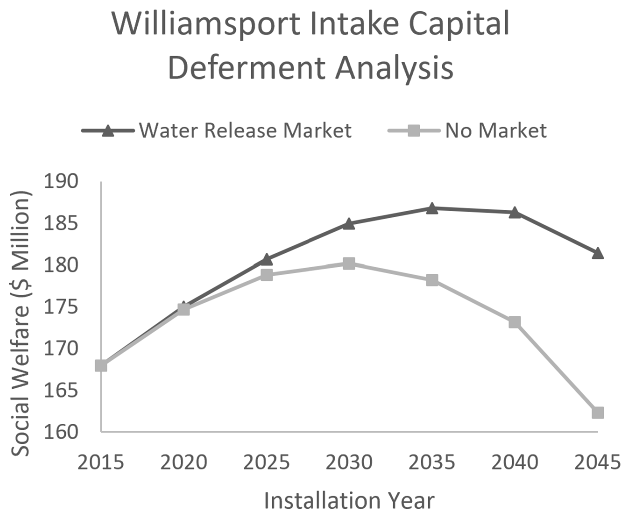


Figure 2.6: Analysis of water-supply project timing for the Duck River Model

converted the annual payment to cost per MGD per planning period.

Figure 2.6 depicts the results of these scenarios. For each scenario, social welfare is plotted against the installation year for both the water release market and the no market models. The water release market is referred to generically because the GCM and CSM models produce identical results. This arises because there are no intermediate players purchasing water. Also, based on Theorem 3, the prices for all upstream nodes of Columbia active in the loss-reduction market must have similar nodal prices (in the GCM formulation). Take for example the year 2025. In that case, Columbia purchases from DRUC, Shelbyville, and Spring Hill, and the resulting, common market price for water is 0.874 (not graphically shown). The curves reveal a trade off between water-use benefits and capital cost savings in terms of the installation year for the project. Furthermore, this trade-off occurs at higher social welfare (i.e., benefits minus costs) for the water release market than the no market model. The water release market also enables the project to be deferred for longer. As noted previously, the cost of the installation decreases the longer it is deferred. However, the cumulative opportunity costs, as measured through γ^{flow}, increase with deferment because less water is available to satisfy economic growth. These competing costs are jointly minimized between the years 2035 and 2040 for the water release market.

The water release market decreases the water opportunity cost to make continued capital deferment viable, thereby serving as a temporary water supply solution. This can be visualized in Figure 2.7, which depicts the estimated flow conditions five years prior to the optimal time frame for the Williamsport Intake installation. The inflow needed to meet water demand is only a limiting factor (i.e., binding constraint) for Columbia because they are the only utility with a non-zero value for $r_{i,t}^{fc}$. To reduce the supply deficit, Columbia purchases a small amount of consumptive-loss reductions from each player to decrease the opportunity cost of deferring the Williamsport Intake project another five years. This can be observed in the differences between the *inflow with market* and *inflow without market* curves.

The Duck River case study reveals a potential unintended consequence of the water release market. Market profits (i.e.,$\pi_{i,t}^{as} - c_{i,c,t}^{cu}$) tend to increase water consumption beyond what it would be otherwise. Table 2.6 demonstrates how profit generated from the water release market (i.e., $\lambda_{i,t}^{sup}$) can increase water consumption. The nominal demand represents the projected water needs, and Q represents the total water withdrawn for consumption. Each of the players upstream of Columbia occasionally use more water than their nominal demand during the Williamsport Intake deferment period (i.e., 2015-2030). Such excess water consumption only occurs when $\lambda_{i,t}^{sup}$ is positive, which can be interpreted as market profits.

Thus, increasing consumption allows the upstream users to experience more consumptive losses and subsequently derive more consumptive loss-reduction revenue from Columbia. All the upstream players that make loss reductions have a positive value for λ^{sup} in 2030. This is when Columbia's water demand opportunity cost is the highest in the deferment period. Several

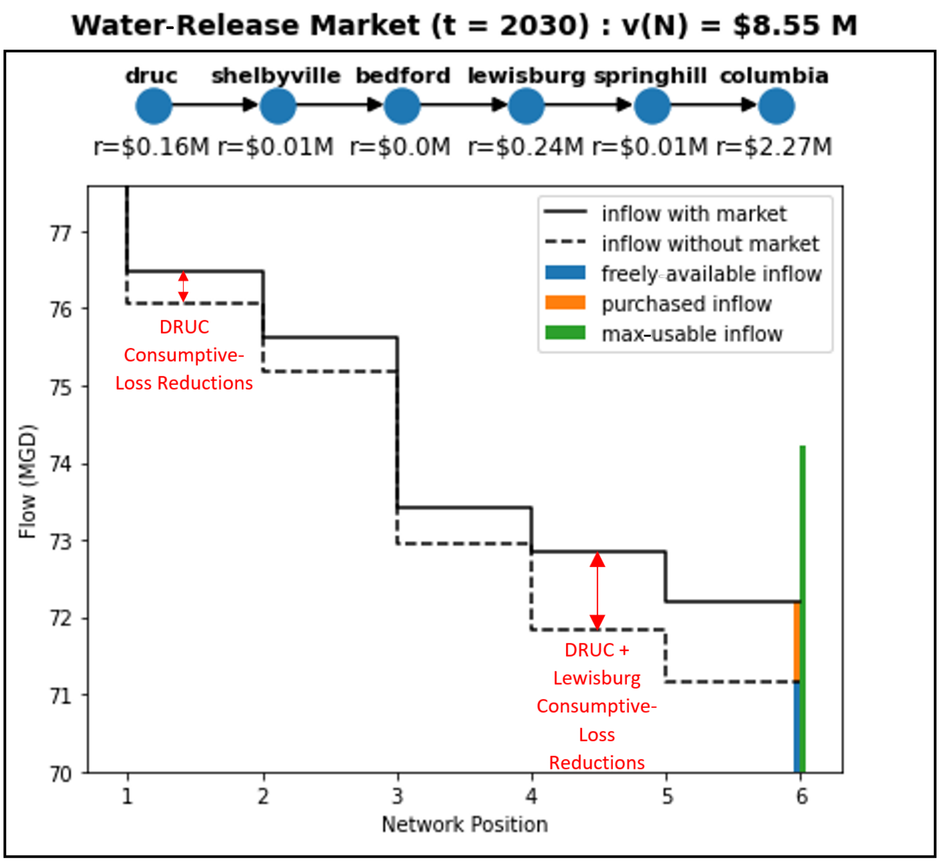


Figure 2.7: Function of the water release market in 2030 (five years before the optimal installation of the capital project)

Table 2.6: Impact of the water-release market on water demand in the Duck River Model

Utility (i)	Time Period (t)	$Q_{i,t}$ (MGD)	Nominal Demand (MGD)	$\lambda^{sup}_{i,t}$ (\$ M)
DRUC	2030	7.5	7.27	0.06
Shelbyville	2015	3.98	3.85	0.07
Shelbyville	2030	5	4.89	0.03
Lewisburg	2015	2.59	2.47	0.06
Lewisburg	2030	3.27	3.17	0.03
Spring Hill	2015	2.79	2.66	0.06
Spring Hill	2030	3.95	3.84	0.03

players also have positive values for λ^{sup} in 2015 because consumptive losses occur at lower rates for these players in later time periods.

2.6 Conclusions

The river basin equilibrium formulations presented reveal a general framework for non-cooperative models on line graphs. In the three-node example, a market structure leads to non-negative rewards for all players. However, these models are needed to determine which market structure is necessary to achieve these rewards. In the Duck River example, the water-release market acts as a temporary solution to help optimally defer capital investments. In all cases, it was assumed that consumptive-loss reductions are practical and relatively cheap to implement. Water releases from storage become much more important when this assumption fails.

Future research will build on the water-release market approach to make it more versatile for more types of river basins. For example, the models in this chapter assume that upstream players cannot completely control the water resource. This assumption could fail in situations with few players or restricted water access. In such a case, treating the river basin as a Stackelberg game is perhaps more appropriate. An alternate bi-level formulation could consider the top level player as a government entity that imposes regulatory flow constraints on the lower level players. Lastly, considering the role of groundwater could be important in river basins with high agricultural usage.

Chapter 3: Reducing Pollution in River Systems using a Stochastic, Game-Theoretic Modeling Approach

3.1 Motivation

In the United States, the total maximum daily load (TMDL) serves as the primary metric used to characterize pollutant-impaired water bodies. It is a calculation of the maximum amount of a pollutant allowed to enter a water body so that the water body will meet and continue to meet water-quality standards [55]. TMDLs are said to be implemented when enough investments are made to bring the pollutant loadings within the allowable amount. Benham et al. (2016) surveyed seventeen separate case study watersheds with successful TMDL implementations [56]. The authors identified three important challenges that must be overcome to achieve a successful implementation:

1. Procuring necessary funding for pollution-reduction investments
2. Improving communication and coordination among local agencies
3. Acquiring sufficient data to characterize the watershed and pollutant sources

An example of item #1 relates to funding the Washington, DC Clean Rivers program. This program has involved extensive investment in infrastructure to reduce combined-sewer overflows into DC's waterways [57]. Financing these infrastructure improvements led to an increase in stormwater fees for churches and other non-profit organizations. In response, DC leaders implemented a $13 million relief program to maintain the necessary funding in a more equitable manner [58].

As an example of item #2, nutrient trading of nitrogen and phosphorus water pollution is currently practiced in the United States [59]. The purpose of this trading is to use market mechanisms to find a cost-effective solution to achieve water-quality goals. Specifically, it allows pollutant generators with a high cost of compliance to purchase credits to achieve their regulatory requirements. These credits are generated as compensation for pollutant generators that simultaneously increase their pollution-reduction requirements. This compliance approach has been a major factor in the elimination of nearly 2.5 million pounds of nitrogen to the Chesapeake Bay from Virginia waters in 2011 [36].

In terms of item #3, the degree of water pollution is inherently uncertain (i.e., stochastic) because weather and human activity ultimately drive the fate and transport of pollutants throughout a river basin. Fortunately, smart infrastructure technologies can help to increase the availability of water-quality data and to statistically characterize this uncertainty. The enabling technologies include remote sensing, machine learning, the "internet of things", and cloud computing. The Digital Anacostia concept is an example of an effort to integrate this information together for improved decision-making [60].

Addressing these three challenges almost always requires an implementation plan that is specific and realistic to the watershed [56]. Therefore, the focus of this chapter is to present a modeling framework to assist with the development of such implementation plans. Section 3.2 covers the relevant literature pertaining to this topic, while Section 3.3 highlights the specific research contributions of this chapter. Section 3.4 sets forth the relevant mathematical theory, which is then formulated as a specific model in Section 3.5. Section 3.6 applies this model to a stylized river basin to motivate the features and the expected benefits of the model. Section 3.7 presents a case study of the approach to the Anacostia watershed in metropolitan Washington, DC. Lastly, in Section 3.8, a conclusion is provided with suggestions for future research.

3.2 Literature Review

The StormWISE-TMDL model [61] is foundational to the model developed in the current chapter. It provides a cost-minimizing solution to achieve water-quality goals. The aspects incorporated into this chapter are described in detail in Section 3.5. The StormWISE-TMDL model was chosen for two reasons. First, StormWISE-TMDL is general enough to be adapted to multiple types of pollutants. The primary assumption to enable this generality is that pollution-reduction benefits are subject to diminishing returns on investment. This occurs because pollution reduction is typically an aggregate effect of many individual best management practices (BMPs) such as rain gardens. Such practices have distinguishable costs and benefits. This contrasts with other domains that have large fixed costs and small marginal costs.

Second, StormWISE-TMDL exhibits a very desirable property for obtaining optimal solutions. Specifically, StormWISE-TMDL is a convex, linear optimization problem. Such problems have the property that any local solution is actually a global one, which is not necessarily true for non-convex problems. This property provides a guarantee of achieving a global minimum, which represents the set of the best solutions possible given the constraints [62]. This is important for obtaining optimal (infrastructure) decisions. In this context, obtaining the true minimal cost is important to provide realistic funding estimates for pollution mitigation. Thus, this model is well suited to address TMDL Implementation Challenge #1.

In contrast, the other models in the stormwater management literature tend to be either non-convex or restricted to specific pollutants. Limbrunner et al. (2013) formulate a linear program, but the results are limited to stormwater runoff reduction [63]. Sasikumar and Mujumdar (1998) develop a linear program for nutrient transformations within the stream, but the linear program restrictively assumes the absence of pollutant interactions [64]. Most other authors use elements of genetic algorithms to solve non-convex optimization problems [65] [66] [67] [68]. Other approaches that relate to non-convex programming problems in water and land infrastructure include, for example, multi-objective optimization balancing competing stakeholder objectives [69] [70]. As opposed to StormWISE-TMDL, the non-convex formulations represent the non-linear physics of fluid flow and material transport to achieve a higher level of model resolution. However, this accuracy can come at the expense of computational difficulties.

More recently, the state of the art in water-quality modeling has moved away from a pure physical process modeling approach to one that incorporates more statistical analysis. The Chesapeake Assessment Scenario Tool (CAST) is an example of a recent implementation of this approach for the Chesapeake Bay [71]. Specifically, CAST generates pollutant-loading scenarios for a hypothetical BMP portfolio. This approach has also been integrated into a non-convex optimization framework to consider many scenarios in the same decision-making process.

One of StormWISE-TMDL's limitations is that it only accommodates a single decision-maker. Most watersheds are trans-boundary in the sense that multiple jurisdictions control different regions of the watershed. For example, in the Anacostia Watershed of metropolitan DC, three different municipal districts are responsible for a large portion of the stormwater pollution reduction activities. These districts are Washington, DC, Montgomery County, Maryland, and Prince George's County, Maryland. If political structure contributes to sub-optimal coordination, then the watershed is said to have a poor institutional fit. This outcome causes the watershed to suffer as a whole [60].

In cases of poor institutional fit, a single optimization problem may not satisfy TMDL Implementation, i.e., Challenge #2. To address this limitation, adaptive-management schemes have been advanced to provide a more collaborative implementation of pollutant-reduction requirements [72] [35]. As will be shown, this chapter explores a water-quality credit market as the primary, adaptive-management strategy.

Market-based mechanisms are not widely applied to water resource systems, but market drivers exist. Structural differences among river basin users create the potential for price differences of water-related commodities. These commodities flow from the user with the lower price (i.e., seller) to the user with the higher price (i.e., buyer). For example, the upstream to downstream structure of a river has been explored as a potential driver for water supply markets [24], [14].

Recent papers [24], [14] follow a tradition of using non-cooperative game theory to evaluate infrastructure markets. For example, complementarity modeling is a specific form of game theory that has been used to analyze liberalizing electric power and natural-gas markets [21]. It is applicable to many other infrastructure systems as well. This approach is amenable to using convex optimization problems as an input, which is why StormWISE-TMDL is preferred to a non-convex alternative (e.g., CAST). The interactions among the optimizing players helps one understand why the players of the game lack incentives for cooperation. Accordingly, corrective-action policies (e.g., water regulations, market tariffs, etc.) are implemented to address these missing incentives.

Another limitation of StormWISE-TMDL is that the model is deterministic. Hydrology involves a myriad of complex processes with many uncertain parameters that are difficult to estimate at the watershed scale (e.g., soil infiltration processes). Furthermore, the response of the watershed may vary considerably with precipitation intensity, antecedent moisture conditions, and management practices [73]. Thus, to address TMDL Implementation Challenge #3, optimization or equilibrium models should consider the stochastic nature of data obtained from water-quality simulations.

For instance, pollutant fate-and-transport processes are exogenous to StormWISE-TMDL. They are implicitly considered in the required pollutant-reductions from land areas. This modeling decision fits quite naturally with the TMDL program because water-quality regulations are expressed in terms of pollutant quantities instead of desired in-stream concentrations [55]. However, the simulation models used for this purpose often have excessive margins of safety (MOS). In response, the National Research Council suggested that the EPA end the arbitrary selection of the MOS and require uncertainty analysis as the basis for MOS determination [74]. Probability network models have been used as the basis for such an uncertainty analysis [75]. They model the dynamics of joint probability distributions and are used to infer the values of random parameters given observed values [76].

BMPs are implemented to achieve pollution reductions, but BMP performance is subject to significant uncertainty. Stormwater BMP databases, which have become available in recent years, help with estimating costs and treatment efficiencies [77]. However, these metrics vary considerably according to site-specific factors that are difficult to classify. One approach to address BMP performance uncertainty uses a two-stage stochastic programming framework with

Bayesian inference [78].

3.3 Contributions of this Chapter

This chapter posits that none of the existing modeling frameworks in the operations research literature simultaneously address all three of the TMDL implementation challenges described in [56] for river systems. While StormWISE-TMDL does address Challenge #1, the model in this chapter extends StormWISE-TMDL into a stochastic, game-theoretic setting using equilibrium programming techniques via a mixed complementarity problem (MCP) formulation. Players within the watershed each solve their own optimization problems for optimal BMP investments. However, players may trade credits for water-quality improvements to achieve a more cost-effective implementation. This trading approach addresses Challenge #2. Pollutant loading uncertainty is considered using chance constraints [79] in each player's optimization problem. These constraints address Challenge #3. For these reasons, this chapter refers to the model herein as TMDL-C3.

Lastly, this chapter conceptualizes water resources using a systems perspective. The purpose of this approach is to appeal to as many multi-disciplinary audiences as possible, which the ubiquity of water resources demands. As such, the Systems Modeling Language (SysML) [1] is used in many of the figures to graphically illustrate the key features of the problem setting and the model. For unfamiliar readers, a symbolic dictionary is provided in Figure 3.1.

Symbol	Name	Description	Examples
<<block>> **[Name]**	Block	A fundamental entity in the systems model. Blocks serve as the basis for definitions and instances of those definitions in a system model.	watershed, land surfaces, river segments
	Decomposition relationship	A type of relationship between two blocks where the block on the arrow end can be considered as ***part of*** the block on the diamond end.	Land surfaces and stream segments are ***part of*** a watershed.
	Generalization relationship	A type of relationship between two blocks where the block that contacts the line endpoint can be considered as a ***type of*** the block on the end with the open triangle.	Nitrogen is a ***type of*** pollutant.
	Dependency relationship	A type of relationship between two blocks where changes to one block necessitates changes to the another.	The watershed improvement plan is dependent on the TMDL requirements.
	Item Flow	An extensive quantity of mass, energy, or information that flows between two parts of a block.	flow of water or pollutant
	Port	A part of a block that serves as a point of exchange for an item flow. The direction indicates the valid directions of flow.	inlet or outlet to a stream

Figure 3.1: SysML symbolic dictionary [1]

3.4 Mathematical Theory

TMDL-C3 can be understood as a specific instance of a particular integration of mathematical modeling techniques. These techniques and their relationships to one another are summarized in Figure 3.2. Accordingly, this section describes these techniques and the associated relationships in sufficient detail to orient the reader to the applicable theory in TMDL-C3. Section 3.5 specializes the theory in this section to the water-related system under consideration.

3.4.1 Equilibrium Programming

Most generally, TMDL-C3 is a specific type of a game-theory model known as an equilibrium program. These programs are characterized by their solution sets, known as Nash equilibrium (NE) points. These solutions reflect situations where all the players have no incentive

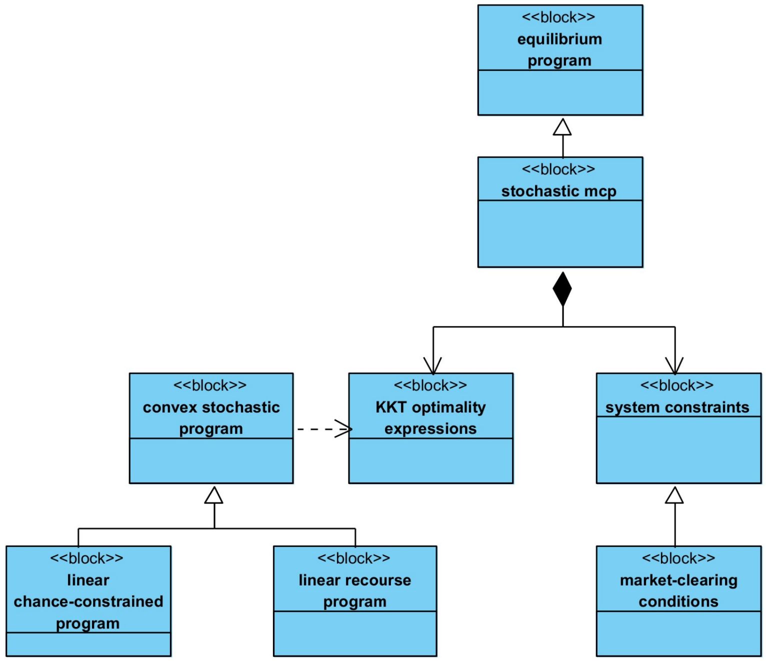


Figure 3.2: General conceptual structure underlying the mathematics of TMDL-C3

to deviate from their strategies. In institutional settings (e.g., water utilities), NE can mathematically explain a status quo of behaviors in terms of how certain incentives could lead actors to choose certain actions. Thus, these solutions can serve an important role in policy analysis.

Assume that the strategies of player $p \in P$ can be represented by a convex, mathematical program of the following form:

$$\min f_p(x_p) \tag{3.1a}$$

$$\texttt{s.t.}$$

$$g_{p,i}(x_p) \leq 0 \quad , \quad i = 1, ..., m_1^p \quad (u_{p,i}) \tag{3.1b}$$

$$h_{p,j}(x_p) = 0 \quad , \quad j = 1, ..., m_2^p \quad (v_{p,j}) \tag{3.1c}$$

where the p subscript is for player p and its set of decision variables is given by $x_p \in \Re^{n_p}$ [1]. The terms u and v are Lagrange multipliers, which have the same meaning as defined in Chapter 1. A solution to an equilibrium program follows from each player optimizing their own version of (3.1) simultaneously. To give a water example, this program could be to determine the lowest-cost BMP strategy subject to TMDL loading limitations. The specific mathematical program considered in TMDL-C3 is provided in Section 3.5.3.

Program (3.1) can be re-expressed via the Karush-Kuhn Tucker (KKT) optimality conditions:

For each $p \in P$, find the vectors $\bar{x}_p, \bar{u}_p, \bar{v}_p$ s.t.:

$$\nabla f_p(\bar{x}_p) + \sum_{i=1}^{m_1^p} \bar{u}_{p,i} \nabla g_{p,i}(\bar{x}_p) + \sum_{j=1}^{m_2^p} \bar{v}_{p,j} \nabla h_{p,j}(\bar{x}_p) = 0 \tag{3.2a}$$

$$g_{p,i}(\bar{x}_p) \leq 0 \quad , \quad \bar{u}_{p,i} \geq 0 \quad , \quad g_{p,i}(\bar{x}_p) \perp \bar{u}_{p,i} \quad , \quad i = 1, ..., m_1^p \tag{3.2b}$$

$$h_{p,j}(\bar{x}_p) = 0 \quad , \quad \bar{v}_{p,j} \quad free \quad , \quad j = 1, ..., m_2^p \tag{3.2c}$$

where $g_{p,i}(\bar{x}_p) \perp \bar{u}_{p,i} \equiv \bar{x}_p \bar{u}_{p,i} = 0$. The specific KKT conditions in TMDL-C3 are provided in Section 3.5.5.

Additional system constraints, such as market-clearing conditions, are used to govern the interactions among the players. To represent these mathematically, consider an q-dimensional [2] system of equations of the following form:

$$\Gamma_k(x) = 0 \quad , \quad \pi^{sys} \quad free \quad , \quad k = 1, ..., q \quad , \quad x = [x_1^T, ..., x_{|P|}^T]^T \tag{3.3}$$

[1] The terms n_p,m_1^p, and m_2^p are positive integers that are arbitrary and problem specific.
[2] q is a positive integer that is arbitrary and problem specific.

In words, let Γ be a function that determines some additional vector π^{sys}. This function takes the union of all the player's decisions as an argument. Crucially, the components of π^{sys} are not decision variables in (3.1) for any player p. However, they can represent parameters that the players must consider in their optimization problems. For example, π^{sys} could represent a vector of prices. The specific system constraints in TMDL-C3 are provided in Section 3.5.6.

A mixed complementarity problem (MCP) can be used to create an equilibrium; it is a nonlinear system of the following general form:

$$0 \leq F_i(\mathbf{x}, \mathbf{y}) \quad \forall i \tag{3.4a}$$

$$\mathbf{x}_i \geq 0 \quad , \quad i = 1, ..., n_1 \tag{3.4b}$$

$$F_i(\mathbf{x}, \mathbf{y})\mathbf{x}_i = 0 \quad , \quad i = 1, ..., n_1 \tag{3.4c}$$

$$F_i(\mathbf{x}, \mathbf{y}) = 0, \quad \mathbf{y}_i \quad free \quad , \quad i = n_1 + 1, ..., n \tag{3.4d}$$

where $F : \Re^n \to \Re^n$ is a generic function of the $\mathbf{x} \in \Re^{n_1}$ and $\mathbf{y} \in \Re^{n_2}$ vectors ($n = n_1 + n_2$). In the equilibrium programming setting, F includes expressions that represent either each player's behavior under uncertainty or expressions governing their interactions (e.g., market clearing constraints). Each component of $\mathbf{y}$ is free to take on any value on the real number line (as indicated by *free* in (3.4d)). The mathematical relationship between F_i and $\mathbf{x}_i$ in Expression (3.4c) is called a complementarity relationship, which corresponds to (3.2b) in the KKT conditions. Concatenating Equations (3.2) and (3.3) results in the specific form of F that applies to the work in this chapter:

$$F\begin{pmatrix} x \\ u \\ v \\ \pi^{sys} \end{pmatrix} = \begin{pmatrix} \nabla f_p(x_p) + \sum_{i=1}^{m_1^p} u_{p,i} \nabla g_{p,i}(x_p) + \sum_{j=1}^{m_2^p} v_{p,j} \nabla h_{p,j}(x_p) \quad , p = 1, .., |P| \\ -g_{p,i}(x_p) \quad , p = 1, .., |P| \quad , \quad i = 1, ..., m_1^p \\ h_{p,j}(x_p) = 0 \quad , \quad j = 1, ..., m_2^p \\ \Gamma_k(x) \quad , \quad k = 1, ..., q \end{pmatrix} \tag{3.5}$$

This particular equilibrium program formulation, which uses the aforementioned MCP theory, is quite broad and has been applied to a number of game theoretic problems [24], [14], [80], [21], [81], [15], [20], [82].

3.4.2 Chance Constraints

If Program (3.1) has uncertain parameters, one must make additional assumptions on the components of f,g, and/or h. Multi-stage stochastic programming and chance-constrained programs [83] are often used for problems with uncertain parameters that can be characterized with probability distributions. The primary difference between these two approaches is related to whether or not decisions can be made after the uncertainty resolves (i.e., if there is any recourse). The underlying probability distributions can either be discrete or continuous, depending on the specific assumptions of the problem setting.

In multi-stage programming, some decisions are made before the values of uncertain parameters become known. These are known as first-stage decisions and allow for the hedging of multiple uncertain scenarios. Once the uncertain parameters are revealed, then follow-up (i.e., recourse) decisions are made in the second stage. As an example, consider a water treatment planning problem. The first stage decision could be deciding the size of the plant to build for uncertain demand. The recourse decision could be selling unused water to another utility. The interested reader can refer to [83] for mathematical details.

In chance-constrained programming, one assumes that recourse actions are not possible. Thus, the decisions that are made are fixed and do not change from scenario to scenario. The inequalities of g may not be satisfied in every scenario because the decisions are fixed, yet the actual parameter values of g can still vary. Consequently, chance constraints are expressed in terms of a necessary reliability such that the constraint is satisfied for a certain percentage of uncertain-parameter realizations. This percentage is specified as a model input.

Chance-constrained programming is the stochastic programming approach used in TMDL-C3. In this chapter, the decisions represent the installation of pollution-reduction technologies, while the chance constraints represent the actual water pollution generated. This formulation is appropriate because there is little recourse once the pollution is released into the environment. However, investing in sufficient technologies can make water quality more reliable in the long run.

Specifically, the chance constraints in TMDL-C3 have the following mathematical form:

$$P(\{\xi | a_{p,i}(\xi)x_p \geq b_{p,i}(\xi)\}) \geq \alpha_i, \quad i = 1, ..., m_1^p \tag{3.6}$$

where $a_{p,i}$ is the ith row of a matrix A_p with uncertain elements, and $b_{p,i}$ is the ith component of a random vector b_p. The term denoted as ξ is a random parameter, which determines the specific realizations of A_p and b_p. The term α_i, which is data, specifies the required reliability level for each constraint. These are denoted as linear chance-constraints because each component of x_p is multiplied by a scalar coefficient. However, it may be necessary to transform these linear chance constraints to non-linear expressions. These chance constraints are also separable because no joint reliability is specified for all the constraints together.

$P(.)$, prevents Equation (3.6) from being used directly in a mathematical program. Fortunately, the following assumptions are sufficient to obtain a deterministic equivalent.

Assumption 1. *ξ is distributed such that the vector $[a_{p,i}(\xi), b_{p,i}(\xi)]$ is jointly normally distributed with mean $[\bar{a}_{p,i}(\xi), \bar{b}_{p,i}(\xi)]$ and a variance-covariance matrix V.*

Assumption 2. *The reliability must be greater than 50% for each constraint (i.e., $\alpha_i \geq 0.5 \quad \forall i \in \{1, ..., m_1^p\}$).*

If these assumptions are satisfied, Equation (3.6) can be re-expressed as follows [84]:

$$\mu(x_p) + \Phi^{-1}(1 - \alpha_i)\sigma(x_p) \geq 0 \tag{3.7a}$$

where Φ^{-1} is the quantile of the standard normal cumulative distribution function, and both μ and σ are short-hand expressions for the following summary statistics:

$$\mu(x_p) \equiv \bar{a}_p x_p - \bar{b}_p \tag{3.7b}$$

$$\sigma(x_p) \equiv \sqrt{[x_p^T, -1]V[x_p^T, -1]^T} \tag{3.7c}$$

where the row superscript i is dropped for parsimony.

Several observations can be made regarding (3.7). Expression (3.7a) is a second-order-cone constraint [85], whose feasible region is convex. Thus it can be incorporated into $g_{p,i}$ in

Equation (3.5) as part of the sufficiency KKT conditions. When α_i = 0.5, then Φ^{-1} is equal to zero and the problem reduces to a deterministic, linear program based on the average values of the random parameters. The specific deterministic equivalent in TMDL-C3 is provided in Section 3.5.4. Secondly, the vectors with -1 as components in (3.7c) are used to allow the covariances of terms involving b_p to be considered in the deterministic equivalent. This works because the expression $\sum_{j=1}^{n_p} a_{p,j}x_{p,j} \geq b_p$ can be rewritten as $\sum_{j=1}^{n_p+1} a_{p,j}x_{p,j} \geq 0$ with $a_{p,(n_p+1)} = b$ and $x_{(n_p+1)} = -1$ [86].

3.5 TMDL-C3 Formulation

This section describes how TMDL-C3 translates the theory of the previous section into an application to address the TMDL implementation challenges. TMDL-C3 is a specific instance of the general program (3.5) that has chance constraints as described in Section 3.4.2. The sets, variables, and parameters of this Section are summarized in Appendix B.1, B.2, and B.3, respectively.

3.5.1 Modeling Approach

In river systems, the TMDL is developed to reduce the delivery of potentially harmful water-quality constituents $c \in C$ to stream segments in the watershed. The set C often includes sediment, bacteria, nitrogen, and/or phosphorus. The first two pollutants (sediment and bacteria) are common because of design limitations and deterioration of urban drainage systems. The second two pollutants (nitrogen and phosphorus) are common because of runoff from fertilized land (agricultural or urban). In general, constituent c is considered a pollutant if it causes an adverse impact to humans or aquatic life. For example, sediment can lead to cloudy water that blocks sunlight to aquatic plants. Nutrients can lead to algal blooms that are toxic to aquatic species and recreational users.

Land segments are usually the source of the excess delivery of a given pollutant c. It is carried in runoff to the stream segment. The magnitude of a given pollutant c can vary according to the land use type $l \in L$. The set L often includes paved urban areas, forests, and agricultural land. Natural characteristics of the sub-watershed $w \in W$ also introduce variation; this is because of varying topography and soil properties across the watershed.

Player $p \in P$, which is a local municipal government, must choose one or more treatment technologies $t \in T$ to reduce pollution within their jurisdictional boundary. An implicit governance structure, such as a pollution-control agency, upholds the pollution-reduction requirements. The set T is usually a collection of best management practices (BMPs) such as pervious pavement, bioretention, etc. The boundary of player p's jurisdiction need not be aligned with a particular sub-watershed or land use. Because of this, each land segment in the watershed is indexed by the Cartesian product of P, W, and L (respectively players, sub-watersheds, land-use categories).

The structure of TMDL-C3 can be best understood in terms of TMDL implementation vs. TMDL development. The governance entity develops the TMDL and enforces it. The set of players P then implement the TMDL as a collective regulatory requirement. The TMDL development process is principally focused on *in-stream* pollutant concentrations and the impacts to aquatic life in the stream. In contrast, TMDL implementation is concerned with reducing the mass and/or volume of *pollutant loadings* from outside the stream. Consistent with the theme of this chapter, the scope of TMDL-C3 applies to the implementation phase.

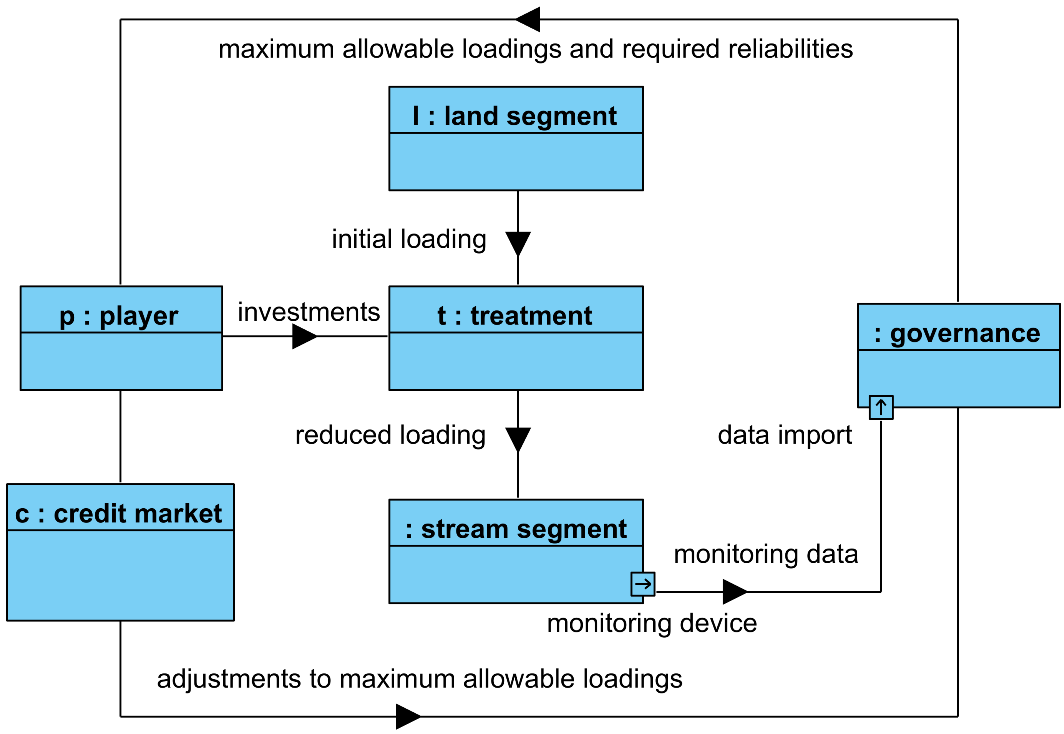


Figure 3.3: TMDL-C3 context and schematic

TMDL development is shown on the right side of Figure 3.3. The governance structure usually develops a separate water-quality model (not shown here) to understand how pollution impacts the stream or water body of interest. The primary data inputs to this model are derived from in-stream monitoring of flow rate and constituent concentrations. The impacts are determined in reference to biological endpoints such as fish populations and predictor variables of healthy waterways such as turbidity [3] and nutrient concentrations. A variety of pollution-reduction scenarios are run in the aforementioned water-quality model to determine player p's maximum allowable loading (i.e., outflow) of constituent c to the watershed, $o_{p,c}^{allw}$. Additionally, $\alpha_{p,c}$ specifies the required reliability level for the allowable loading. In current practice, $\alpha_{p,c}$ is usually based on an average loading. However, $\alpha_{p,c}$ is allowed to vary in this chapter. The colons without letter codes in the governance and stream segment blocks indicate that these features are

[3] Turbidity is a measure of the amount of scattering of light in a water source. It is an indicator of water clarity.

not modeled as an explicit set in TMDL-C3.

TMDL implementation, following TMDL development, is shown on the left side of Figure 3.3. To meet the maximum allowable loadings, player p will decide a series of investments $I_{p,t,w,l}$ to treat land segment p, w, l with technology t. The parameters $i^{up}_{p,t,w,l}$ represent upper bounds on these investments due to site constraints. Technically speaking, land segment p, w, l generates an initial loading, which technology t prevents from reaching the water body. The reduced loading represents the quantity of pollution that bypasses technology t.

TMDL implementation is subject to uncertainty in constituent loadings and BMP effectiveness. Fortunately, probability distributions, which are denoted using hat notation (ˆ) can often be used to characterize such uncertainty. Let $\hat{o}^{init}_{p,c}$ denote player p's initial loading (i.e., outflow) of constituent c to the stream segments in the watershed across all land l. This quantity is treated as a random parameter. In accordance with StormWISE-TMDL, this chapter assumes that the reduction in the loading is directly proportional to $I_{p,t,w,l}$. The associated proportionality constant is denoted as $\hat{s}_{p,c,t,w,l}$, which is also treated as a random parameter. Motivation for treating these terms as random parameters is given in Section 3.5.2.

TMDL-C3 does not eliminate uncertainty but does separate it into its component parts: aleatory uncertainty and epistemic uncertainty. The former (denoted with the hat symbol) refers to uncertainty that is empirical in nature and can reasonably be described with probability distributions [87]. Thus, this model represents this uncertainty endogenously via $\hat{o}^{init}_{p,c}$ and $\hat{s}_{p,c,t,w,l}$. The latter refers to uncertainty that is fundamentally related to a lack of knowledge [87]. For example, this uncertainty is often related to the uncertain impacts of pollution on aquatic environments, which can be handled using Bayesian inference methods [75]. However, Section 3.6 demonstrates how sensitivity analysis can be used to provide a simple yet lucid characterization of epistemic uncertainty.

In this chapter, TMDL-C3 uses a credit market as an adaptive-management strategy. The key market driver in this setting is related to how differences in land characteristics translate into differences in BMP cost effectiveness. This land heterogeneity is primarily a function of pollution concentration. For example, BMPs to reduce nitrogen are likely most effective where the this type of pollution is high. A farm would likely have more nitrogen to be reduced than a paved urban area because of the fertilizer used on crops. A stylized watershed featuring aspects of these urban / rural differences is presented in Section 3.6.

Figure 3.3 provides a schematic overview of this market. A supply of credits, $K_{p,c}$ is generated whenever player p reduces more of constituent c than required to meet their allowable loading, $o_{p,c}^{allw}$. This allowable loading is treated as input (i.e., exogenous) data to the problem. Another player can then purchase these credits at a price π_c to reduce their $o_{p,c}^{allw}$ by the amount purchased. Like a traditional market, demand cannot exceed supply. Otherwise, the overall pollution-reduction goals identified during TMDL development would not be met. The mathematical details representing this market are presented in Section 3.5.6.

With this context in mind, TMDL-C3 is developed at an appropriate scale for policy evaluation and building infrastructure investment portfolios. Most engineering details, such as project costs and BMP efficiencies, are treated as exogenous. Many engineering planning and design details are omitted because they are not expected to impact the investment mix in the portfolio. For example, time periods are not considered in this model as only the steady-state production of pollution on an annual basis is considered. Previous literature provides guidance on how to translate steady- state, pollutant-reduction goals into a portfolio of engineering design projects [61].

Table 3.1: Summary of TMDL-C3 parameters and their derivations

Parameter	Calculated from	Anacostia Case Study Data Sources (Section 3.7)
Benefit slopes ($\hat{s}_{p,c,t,w,l}$)	$\hat{e}$,$\hat{r}$,c^{site}	Water-quality model (Section 3.7.1.4), literature (Table 3.5)
Initial loadings ($\hat{o}_{p,c}$)	$\hat{e}$, a^{land}	Water-quality model (Section 3.7.1.4)
Investment upper bounds ($i^{up}_{p,t,w,l}$)	c^{site}, f, a^{land}	Literature (Section 3.7.1)
Allowable loadings ($o^{allw}_{p,c}$)	Scenario values (Table 3.3, Section 3.7)	Literature (Section 3.7.1)
Pollution-reduction reliability ($\alpha_{p,c}$)	Scenario values (Table 3.3, Section 3.7)	Literature (values depicted in Figure 3.11)

3.5.2 Parameter Derivations

The primary parameters of TMDL-C3 are derived from characteristics of the watershed and the technologies under consideration. In Section 3.6, illustrative values are assigned to these parameters. In Section 3.7, these parameters are derived from a water-quality model and relevant literature. Table 3.1 summarizes the TMDL-C3 parameters and their derivations. This table also refers the reader to the locations in the chapter that describe the data sources for these parameters.

The weather drives the aleatory uncertainty in the initial loadings, $\hat{o}^{init}_{p,c}$, and the benefit slopes, $\hat{s}_{p,c,t,w,l}$. Variable rainfall, temperature, and humidity determine the quantities of water flowing and being stored within a watershed. Likewise, water-quantity characteristics affect water quality because of water's capacity to mobilize and store constituents. Thus, the initial loadings of constituents are uncertain, and consequently, so are the benefits of investments to reduce said loadings.

In TMDL-C3, the interdependent relationships of weather, hydrology, and constituent loads are represented using quantities called export coefficients. They represent the annual amount of constituent c generated per unit area in sub-watershed w and land use l. Typically, water-quality simulations are used to estimate export coefficients. TMDL-C3 further distinguishes between two types: the initial-loading export coefficient, $\hat{e}_{p,c,w,l}$, and the reduced-loading export coefficient, $\hat{r}_{p,c,t,w,l}$. Both export coefficients have units of tons/year/hectare. The former is the export coefficient for a land segment without any treatment technologies. The latter represents the same land segment with treatment t installed.

The initial loadings $\hat{o}^{init}_{p,c}$, and the benefit slopes, $\hat{s}_{p,c,t,w,l}$, are derived from the export coefficients. The parameter $\hat{s}_{p,c,t,w,l}$ (tons/\$) is the marginal benefit divided by the marginal cost of BMP installation:

$$\hat{s}_{p,c,t,w,l} \equiv \frac{\hat{e}_{p,c,w,l} - \hat{r}_{p,c,t,w,l}}{c^{site}_{p,t,w,l}} \tag{3.8}$$

The marginal benefit of t, which is the numerator of Expression (3.8), is the difference between the initial-loading export coefficient and the reduced-loading export coefficient for a particular land segment in tons/year/hectare. The marginal cost is simply the parameter $c^{site}_{p,t,w,l}$ (\$/hectare). The initial pollutant loadings are similarly obtained as follows:

$$\hat{o}^{init}_{p,c} = \sum_{w \in W} \sum_{l \in L} \hat{e}_{p,c,w,l} a^{land}_{p,w,l} \tag{3.9}$$

where $a^{land}_{p,w,l}$ is the land area in hectares. In words, player p's initial loading for constituent c (tons/year) equals the sum of pollutants generated across all land use types and all sub-watersheds.

Each random parameter is assumed to be normally distributed. This assumption alludes to the Central Limit Theorem [88] because each random parameter is a weighted sum of export coefficients. Furthermore, the annual export coefficients can be understood themselves as a sum of daily export coefficients. Regardless of the daily export coefficients' distributions, the random parameters will be approximately normally distributed if their daily values are independent and identically distributed. Numerical justification for the assumption of normality is provided in Section 3.7.1.

In contrast with the previous parameters, the upper bound for each investment $I_{p,t,w,l}$ is not modeled as a random parameter. Instead, it is a static estimate related to the siting limitations of a particular treatment technology. For example, it would be practically impossible to replace every parking lot in a watershed with pervious pavement. Setting an upper bound equal to zero covers the case where a technology is never appropriate for a type of site. For example, pervious pavement would probably never be installed in a forest solely for runoff reduction.

These upper bounds are expressed mathematically as follows [77]:

$$i^{up}_{p,t,w,l} = c^{site}_{p,t,w,l} \times f_{p,t,w,l} \times a^{land}_{p,w,l} \tag{3.10}$$

where $f_{p,t,w,l}$ represents the fraction of a given land segment that can be treated with technology t. The product $f_{p,t,w,l} \times a^{land}_{p,w,l}$ represents the area of land that is suitable for the BMP. Multiplying this land area by the marginal cost yields the maximum possible investment for the given BMP.

3.5.3 Formulation for Each Player

As shown in (3.11), each player seeks to minimize the costs of BMP installation (i.e., $\sum_t \sum_w \sum_l I_{p,t,w,l}$) and credit purchases (i.e., $\sum_c \pi_c K_{p,c}$) subject to minimum pollutant-reduction levels. The variables in this program are classified as either "primal" or "dual" variables [45]. The primal variables are denoted with capital letters. They represent decisions related to water-quality investments. In contrast, the dual variables (i.e., Lagrange multipliers) are denoted with Greek letters. They are the change in the objective function for a small change in the right-hand side of the constraint. They are shown in parenthesis next to their corresponding constraint.

$$\min_{I_{p,t,w,l},K_{p,c}} \sum_{t\in T}\sum_{w\in W}\sum_{l\in L} I_{p,t,w,l} + \sum_{c\in C}\pi_c K_{p,c} \tag{3.11a}$$

s.t.

$$P\left\{\sum_{t\in T}\sum_{w\in W}\sum_{l\in L} \hat{s}_{p,c,t,w,l} I_{p,t,w,l} + K_{p,c} \geq \hat{o}^{init}_{p,c} - o^{allw}_{p,c}\right\} \geq \alpha_{p,c} \quad (\gamma^{min}_{p,c}) \quad \forall c \in C \tag{3.11b}$$

$$I_{p,t,w,l} \leq i^{up}_{p,t,w,l} \quad (\gamma^{up}_{p,t,w,l}) \quad \forall t,w,l \in T \times W \times L \tag{3.11c}$$

$$I_{p,t,w,l} \geq 0 \quad \forall t,w,l \in T \times W \times L \quad , \quad K_{p,c} \quad free \quad \forall c \in C \tag{3.11d}$$

Equation (3.11a) represents the objective function for each player. It is the sum of the total investments $I_{p,t,w,l}$ considering all BMP technologies, sub-watersheds, and land use types. Additionally, it includes credits purchased from or sold to the market, $K_{p,c}$. The price variable π_c is treated as exogenous data for each player. Thus, the objective function for each player is linear.

Equation (3.11b) states that the pollutant reductions achieved from investments (i.e., benefit) must be greater than or equal to the minimum requirement, $\hat{o}^{init}_{p,c} - o^{allw}_{p,c}$. Crucially, trading TMDL credits increases or decreases the pollutant-reduction requirements for each player. A single set of decisions may not satisfy this inequality universally because of the random parameters involved (i.e., $\hat{s}_{p,c,t,w,l}$ and $\hat{o}^{init}_{p,c}$). Instead, the inequality must hold for $\alpha_{p,c}$ percent of realizations for these random parameters. Stochastic models of this form are called chance-constrained programs [79].

Equation (3.11b) is indexed by constituent to allow the separate consideration of multiple

TMDLs. This approach contrasts with joint chance constrained programs [89], which assign a single reliability requirement to all the chance constraints collectively. Separate chance constraints are not only easier to solve but are more realistic for this problem setting. TMDLs are developed separately for multiple pollutants because each has special considerations and impacts on aquatic environments. For example, reducing sediment delivery to streams may actually decrease water clarity in the form of algal blooms unless excess nutrients are also reduced [90].

As described in Section 3.4.2, the random components of a chance constraint are assumed to be normally distributed. The decision variables in Expression (3.11b) do not violate this assumption as long as $\hat{s}_{p,c,t,w,l}$ is normally distributed as well. This works because a normal distribution is a specific kind of stable distribution [86]. To see this, consider a stable distribution $X \sim P$. In such a case, another distribution , $Z \sim P$, can be obtained using a transformation $Z \equiv \frac{X - C1}{C2}$. The constant $\mathbf{C1}$ represents a shift applied to X, while $\mathbf{C2}$ represents a scaling factor. These scaling factors can be related to specific parameters in TMDL-C3. For the random parameter $\hat{s}_{p,c,t,w,l}$, $\mathbf{C1} = 0$ and $\mathbf{C2} = \frac{1}{I_{p,t,w,l}}$.

As described in Section 3.5.1, $K_{p,c}$ represents an adjustment to the deterministic term $o^{allw}_{p,c}$. Because of this relationship, the coefficient of $K_{p,c}$ is treated as deterministic as well. However, the coefficient of $K_{p,c}$ is still modeled as normally distributed but with a very small standard deviation (i.e., $\mathcal{N}(1, 1 \times 10^{-6})$). This is done to satisfy the normal distribution assumption in Section 3.4.2.

Equation (3.11c) establishes the upper bounds for a specific stormwater investment. It does not include any variables related to pollutant trading. Thus, it is unchanged from StormWISE-TMDL.

Equation (3.11d) establishes the domain for each type of variable. Stormwater investment levels, $I_{p,t,w,l}$, are non-negative because investments are expressed as expenditures. In contrast, stormwater credits, $K_{p,c}$, are free variables (i.e., can be positive, negative, or zero) because they can be either bought or sold. A positive value indicates a purchased credit, while a negative value indicates a sold credit. This convention requires the net credits bought and sold across all players to equal zero.

3.5.4 Deterministic Equivalent for Each Player

Problem (3.11) can be solved if the probabilistic expression (3.11b) is replaced with a deterministic equivalent (DE). This section introduces the required notation and relates the new notation to that described in Section 3.4.2. This section also succinctly states the final deterministic equivalent for this problem setting.

Per Section 3.4.2, the deterministic equivalent for a chance-constrained program has a variance-covariance matrix, V. TMDL-C3 has $|P| \times |C|$ chance constraints, so each variance-covariance matrix in TMDL-C3 is indexed as $V_{p,c}$ accordingly. Each $V_{p,c}$ can be further decomposed into sub-matrices with respect to the uncertain parameters in TMDL-C3, as follows. Let $V^{s^2}_{p,c}$ contain variances and covariances between different t, w, l that are strictly related to $\hat{s}_{p,c,t,w,l}$. Similarly, let $V^{so}_{p,c}$ contain the covariances of each $\hat{s}_{p,c,t,w,l}$ with the random scalar $\hat{o}^{init}_{p,c}$. Lastly, let $v^{o^2}_{p,c}$ be the scalar variance of $\hat{o}^{init}_{p,c}$. For clarity, this decomposition is summarized in Equation 3.12:

$$V_{p,c} = \begin{bmatrix} V^{s^2}_{p,c} & V^{so}_{p,c} \\ & \\ V^{so^T}_{p,c} & v^{o^2}_{p,c} \end{bmatrix} \tag{3.12}$$

The non-scalar sub-matrices can be further decomposed into scalar variance and covariance entries. To do this, the following multi-dimensional indices are introduced: $j \in T \times W \times L$ and $k \in T \times W \times L$. This allows one to refer to $\hat{s}_{p,c,t,w,l}$ more succinctly as either $\hat{s}_{p,c,j}$ or $\hat{s}_{p,c,k}$. The sub-matrix $V^{s^2}_{p,c}$ is organized into $(|T| \times |W| \times |L|)^2$ entries. Each entry in this sub-matrix is denoted as $v^{s^2}_{p,c,j,k}$, which is the variance of $\hat{s}_{p,c,t,w,l}$ (if $j = k$) or the covariance between $\hat{s}_{p,c,j}$ and $\hat{s}_{p,c,k}$ (if $j \neq k$). Similarly, the sub-matrix $V^{so}_{p,c}$ has $|T| \times |W| \times |L| \times 1$ entries. Each entry in this sub-matrix is denoted as $v^{so}_{p,c,j}$, which is the covariance between $\hat{s}_{p,c,j}$ and $\hat{o}^{init}_{p,c}$.

In TMDL-C3, the variance terms in V are primarily derived from precipitation uncertainty. The covariance terms reflect the tendency of precipitation to increase the delivery of pollutants to water bodies regardless of pollutant type or land characteristics. The geometry of watersheds and the properties of water are responsible for these correlations. Watersheds collect water across a large geographic area and convey it to an outlet of a water body. Water is also uniquely capable of transporting multiple constituents simultaneously.

With this new notation in mind, Equation (3.11b) has the following deterministic equivalent for each player, p:

$$\mu_p + \Phi^{-1}(1 - \alpha_{p,c})\sqrt{\sigma^2_{p,c}} + K_{p,c} + o^{allw}_{p,c} \geq 0 \quad (\gamma^{min}_{p,c}) \quad \forall c \tag{3.13a}$$

where in terms of the general deterministic equivalent (3.7):

$$\mu_p = \sum_{j \in T \times W \times L} \bar{s}_{p,c,j} I_{p,j} - \bar{o}^{init}_{p,c} \tag{3.13b}$$

and

$$\sigma^2_{p,c} = \sum_{j\in T\times W\times L}\sum_{k\in T\times W\times L} v^{s^2}_{p,c,j,k} I_{p,j} I_{p,k} - \sum_{j\in T\times W\times L} 2v^{so}_{p,c,j} I_{p,j} + v^{o^2}_{p,c} \quad \forall c \in C \tag{3.13c}$$

where $\bar{s}_{p,c,j}$ and $\bar{o}^{init}_{p,c}$ are the mean values for each random parameter. Equation (3.13c) represents a product expansion of the term $[x_p^T, -1]V[x_p^T, -1]^T$ in (3.7). A clarifying example of this product expansion with three investments (i.e., $j, k \in \{1, 2, 3\}$) is provided in Appendix B.4.

3.5.5 KKT Conditions for each Player

Each player's optimization problem can be expressed using the KKT conditions because the problem is convex. A solution to the KKT conditions is thus a sufficient condition for an optimal solution [21]. These conditions are as follows:

$$0 \le 1 + \gamma^{up}_{p,j} - \sum_{c\in C} \gamma^{min}_{p,c} \Bigg[\bar{s}_{p,c,j} + \frac{\Phi^{-1}(1-\alpha_{p,c})}{\sqrt{\sigma^2_{p,c}}} \Big(v^{s^2}_{p,c,j,j} I_{p,j} - v^{so}_{p,c,j} + \sum_{k\neq j} v^{s^2}_{p,c,j,k} I_{p,k} \Big) \Bigg] \perp I_{p,j} \ge 0 \quad \forall j \in T\times W\times L \tag{3.14a}$$

$$\pi_c - \gamma^{min}_{p,c} = 0 \quad , \quad K_{p,c} \quad free \quad \forall c \in C \tag{3.14b}$$

$$0 \le \sum_{j\in T\times W\times L} (\bar{s}_{p,c,j} I_{p,j}) - \bar{o}^{init}_{p,c} + \Phi^{-1}(1-\alpha_{p,c})\sqrt{\sigma^2_{p,c}} + K_{p,c} + o^{allw}_{p,c} \perp \gamma^{min}_{p,c} \ge 0 \quad \forall c \in C \tag{3.14c}$$

$$0 \le i^{up}_{p,t,w,l} - I_{p,t,w,l} \perp \gamma^{up}_{p,t,w,l} \ge 0 \quad \forall t, w, l \in T\times W\times L \tag{3.14d}$$

In Expression (3.14a), the second term inside the square brackets is component c of the gradient of $\sqrt{\sigma^2_{p,c}}$ multiplied by $\Phi^{-1}(1-\alpha_{p,c})$. A clarifying example with three investments is provided in Appendix B.4.

3.5.6 MCP System Constraints

The system constraints consist of any remaining equations in the MCP that do not arise from the KKT conditions. In TMDL-C3, they function to connect the player's optimization problems together, as in (3.15a), and to allow for notational substitutions, as in (3.15b). These constraints are a special case of the general system (3.3):

$$\sum_{p \in P} K_{p,c} = 0 \quad , \quad \pi_c \quad free \quad \forall c \in C \tag{3.15a}$$

$$\sigma^2_{p,c} = \sum_{j \in T \times W \times L} \sum_{k \in T \times W \times L} v^{s^2}_{p,c,j,k} I_{p,j} I_{p,k} - \sum_{j \in T \times W \times L} 2 v^{so}_{p,c,j} I_{p,j} + v^{o^2}_{p,c} \quad \forall c \in C \tag{3.15b}$$

Equation (3.15a) represents the market-clearing constraints for the stormwater credits. The sum of these variables (i.e., $K_{p,c}$) must equal zero because the credit market can only redistribute the TMDL allocations. It cannot increase or decrease the sum across all the allocations. To make this possible, stormwater credits can take positive or negative values depending on whether the credits are bought or sold, respectively. In accordance with MCP theory, this equality constraint implies that the credit price can either be positive or negative as well. Negative prices would reflect a situation where the producer of the credit would pay another to remove it from the market.

3.5.7 Aggregate Optimization Problem

The aggregate optimization problem reflects a setting where a central planner controls each player's decision variables to optimize some socially beneficial metric [14]. In TMDL-C3, this metric is the minimum investment cost summed across all the players. In contrast to Sections 3.5.1 - 3.5.6, the aggregate optimization problem is not directly part of TMDL-C3. Instead, it creates a point of comparison to evaluate the equity of TMDL-C3's solutions. This comparison is shown in Section 3.7.2. The objective function and constraints of this aggregate problem is expressed as follows:

$$\min_{I_{p,j},K_{p,c}} \sum_{p\in P} \sum_{j\in T\times W\times L} I_{p,j} \tag{3.16a}$$

s.t.

$$\sum_{j\in T\times W\times L} \bar{s}_{p,c,j} I_{p,j} - \bar{o}^{init}_{p,c} + \Phi^{-1}(1-\alpha_{p,c})\sqrt{\sigma^2_{p,c}} + K_{p,c} + o^{allw}_{p,c} \geq 0 \quad \forall p,c \in P\times C \tag{3.16b}$$

$$\sigma^2_{p,c} = \sum_{j\in T\times W\times L} \sum_{k\in T\times W\times L} v^{s^2}_{p,c,j,k} I_{p,j} I_{p,k} - \sum_{j\in T\times W\times L} 2v^{so}_{p,c,j} I_{p,j} + v^{o^2}_{p,c} \quad \forall p,c \in P\times C \tag{3.16c}$$

$$I_{p,t,w,l} \leq i^{up}_{p,t,w,l} \quad \forall p,t,w,l \in P\times T\times W\times L \tag{3.16d}$$

$$I_{p,t,w,l} \geq 0 \quad \forall p,t,w,l \in P\times T\times W\times L \quad , \quad K_{p,c} \quad free \quad \forall p,c \in P\times C \tag{3.16e}$$

The aggregate objective function is the sum of (3.11a) across all players. The credits bought and sold, $\sum_{p\in P}\sum_{c\in C} \pi_c K_{p,c}$, cancel from the objective function. To see this, the credits bought and sold can be re-expressed as $\sum_{c\in C}\sum_{p\in P} \pi_c K_{p,c}$. Factoring out π_c from the inner summation yields the expression $\sum_{c\in C}\pi_c\sum_{p\in P}K_{p,c}$. From Equation (3.15a), $\sum_{p\in P}K_{p,c} = 0 \quad \forall c \in C$. Thus, the credits bought and sold must sum to zero as well.

The aggregate constraints are (3.11b) - (3.11d) except that they are concatenated across all players. This concatenation is indicated with the $\forall p \in P$ symbology in Expressions (3.16b) - (3.16e). Expressions (3.16b) and (3.16c) are the deterministic equivalent of Expression (3.11b) where the reliability level $\alpha_{p,c}$ remains unchanged from TMDL-C3.

Any global optimal solutions to the aggregate optimization problem, if they exist, can be obtained using a non-linear solver for mathematical programs. This is a convex program because both the objective functions and constraints are convex. The objective function (3.16a) is simply a summation of convex objective functions, which is also convex. The aggregate constraints are either linear or second-order cone and thus are convex as well.

3.6 Stylized River Basin

To illustrate the formulation of Section 3.5, consider a stylized model consisting of two players in a single watershed, 'W1'. The w index is dropped for simplicity of notation. Let 'P1' be a municipality with more pollution from urban land (shortened as 'urb') and less pollution from rural land (shortened as 'rur') and let 'P2' be another municipality with the opposite characteristics. Both players 'P1' and 'P2' have 100 hectares of land split equally by land use. The two players are interested in cooperating together to meet the TMDL requirements for both sediment and nitrogen in the local river. P1's majority pollutant is sediment generated from erosive runoff (Q) from paved areas, while P2's majority pollutant is total nitrogen (N) from excess crop fertilizer.

The export coefficients $\hat{e}_{p,c,l}$ characterize the pollution sources in the stylized watershed. Table 3.2 summarizes the average values for these export coefficients. The range between two averages for 'P1' and 'P2', respectively, is a measure of the heterogeneity in the watershed (e.g., $\bar{e}_{1,Q,urb} - \bar{e}_{2,Q,urb} = 1$). The terms of the variance-covariance matrix were all set to 0.1 to simulate how a precipitation event mobilizes many pollutants at once. The values for $\hat{s}_{p,c,t,l}$ were generated using Equation (3.8). Similarly, the values for $\hat{o}_{p,c}^{init}$ were generated using Equation (3.9). The mean and variance-covariance values were then calculated for these parameters.

Table 3.2: Stylized model average export coefficients

Indices			$\bar{e}_{p,c,l}$	
p	c	l	Value	Units
'P1'	'Q'	'urban'	1.5	m^3 / ha / yr
'P1'	'Q'	'rural'	0.375	m^3 / ha / yr
'P1'	'N'	'urban'	1.25	kg / ha / yr
'P1'	'N'	'rural'	5	kg / ha / yr
'P2'	'Q'	'urban'	0.5	m^3 / ha / yr
'P2'	'Q'	'rural'	0.125	m^3 / ha / yr
'P2'	'N'	'urban'	3.75	kg / ha / yr
'P2'	'N'	'rural'	15	kg / ha / yr

Suppose both players can install BMPs to mitigate excess Q and N. For ease of interpretation, assume that each BMP t has a constant pollution removal efficiency $\eta_{c,t}$ for constituent c. In this simplified scheme, the reduced-loading export coefficient is $\hat{r}_{p,c,t,l} = (1 - \eta_{c,t})\hat{e}_{p,c,l}$. Thus, Expression (3.8) reduces to $\hat{s}_{p,c,t,l} = \frac{\eta_{c,t}\hat{e}_{p,c,l}}{c_{p,t,l}^{site}}$. Within this framework, this section considers three types of hypothetical BMPs, which are chosen to illustrate BMP performance trade-offs:

- Type 't1': High Q removal efficiency ($\eta_{Q,1} = 70\%$) and low N removal efficiency ($\eta_{N,1} = 50\%$)
- Type 't2': Moderate Q removal efficiency ($\eta_{Q,2} = 60\%$) and moderate N removal efficiency

($\eta_{N,2} = 60\%$)

- Type 't3': Low Q removal efficiency ($\eta_{Q,3} = 50\%$) and high N removal efficiency ($\eta_{N,3} = 70\%$)

For simplicity, assume that each of these BMPs have the same unit cost ($c^{site}_{p,t,l}$ = \$10K/hectare) and can treat 1/3 of each player's land area ($f_{p,t,l} = 33.\bar{3}\%$).

Three scenarios were run using this approach, which vary according to the allowable loadings, $o^{allw}_{p,c}$, and the reliability level, $\alpha_{p,c}$. The allowable loadings are expressed as a fraction of the initial loadings. The first scenario ($S1$) was developed to illustrate the dynamics of BMP project selection and trading. This scenario used the average values of the random parameters (i.e., $\alpha_{p,c} = 0.5$) to simplify visualization. Two additional scenarios were developed to compare two different approaches for pollution reduction. The second scenario ($S2$) represents stringent pollution-reduction constraints that are also based on average values for the random parameters. Lastly, the third scenario ($S3$) incorporates an extreme year for pollution into the analysis using chance constraints. The specific motivation and details for $S2$ and $S3$ are described in Section 3.6.2. The differences between the parameters in these scenarios are summarized in Table 3.3.

Table 3.3: Stylized model scenarios

Scenario	$o^{allw}_{p,c}$	$\alpha_{p,c}$
S1: Project Selection and Trading Insights	0.49 $\hat{o}^{init}_{p,c}$	0.5
S2: Stringent, Average Constraint	0.44 $\hat{o}^{init}_{p,c}$	0.5
S3: Extreme-Event Chance Constraint	$\hat{o}^{init}_{p,c}$	0.9

3.6.1 Project Selection and Trading Insights

The stylized model provides project selection insights to address Challenge # 1. Figure 3.4 illustrates the benefit curves for Player 1 and Player 2 across the two pollutant types (i.e., sediment and nitrogen). To generate these curves, the investment level, $I_{p,t,w,l}$, was multiplied by the benefit slope, $\hat{s}_{p,c,t,l}$, to obtain the associated pollution reduction. The total pollution reduced over multiple investments was then ordered and expressed cumulatively to represent a plausible sequence of investments. To obtain the order, the benefit slopes were sorted from largest to smallest for the most stringent pollutant.

The sediment generated by Q was found to be the more stringent pollutant because the dual variable $\gamma_{p,Q}^{min}$ was higher than $\gamma_{p,N}^{min}$ for both players. As described in Section 3.5.3, $\gamma_{p,c}^{min}$ represents the change in the objective function for a small change in the allowable loading term (i.e., $o_{p,c}^{allw}$). Thus, this change is more significant to the model's objective function when $c = Q$ for both players. If $\gamma_{p,c}^{min} = 0$, the constraint will be said to be satisfied automatically. This is because there necessarily is slack in this constraint per the complementary slackness principle in convex programming.

The output of this modeling approach can be understood in relation to a greedy heuristic for BMP project selection. This common heuristic is used to prioritize projects in order of the pollution reduced per pound. It is reasonable provided that one of the two conditions are met:

1. One pollutant should dominate the considerations for project selection, or

2. The BMPs should be equally effective for multiple pollutants

In all other cases, one could expect trade-offs between dollars invested and pollutants reduced.

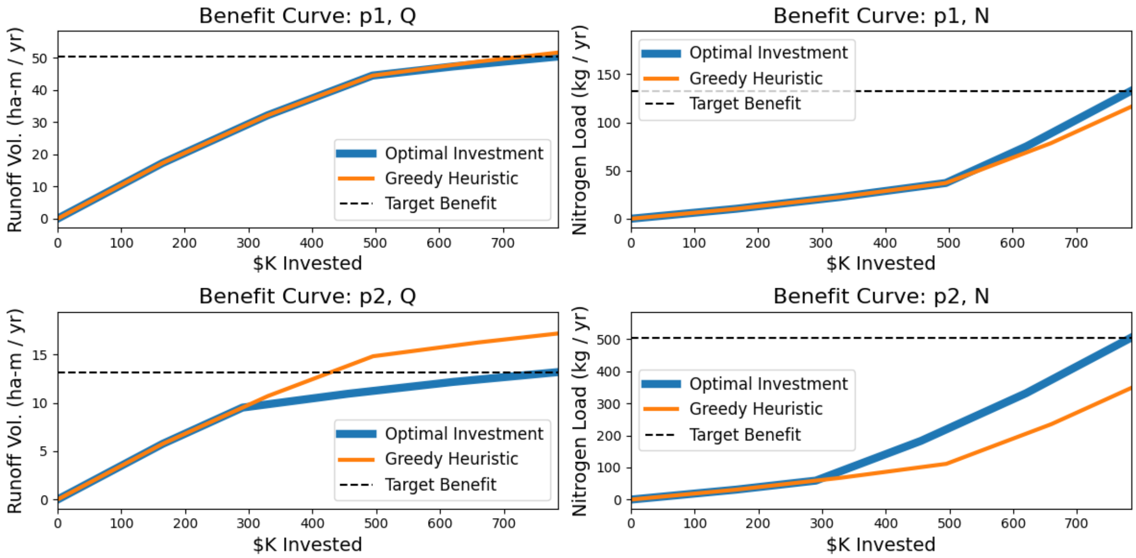


Figure 3.4: Visualization of project selection insights

Figure 3.4 depicts the nature of these trade-offs for the stylized model. For Player 1, the benefit curve for sediment generated by Q matches the greedy heuristic rather closely. This matches an intuitive expectation that the marginal benefits of pollution-reduction investments decrease with increasing scale. Additionally, the greedy heuristic in terms of Q nearly meets the target benefit, $\hat{o}^{init}_{p,c} - o^{allw}_{p,c}$, for total nitrogen, N, automatically. In contrast, Player 2 only satisfies roughly half of the N pollution reduction requirements with the greedy heuristic (see orange curve in bottom right frame). This explains why the optimal investment includes some of the highest performing BMPs for Q but also includes high performing BMPs for N. This also explains the difference in runoff volume between the optimal investment and the greedy heuristic in the lower left-hand frame of Figure 3.4.

The stylized model also provides credit-trading insight to address Challenge #2. Figure 3.5 superimposes the benefit curves that were shown in Figure 3.4 with curves representing the credit market. These latter curves express the relationship between the dollars invested in the market for pollutant c and player p's credit purchases, $K_{p,c}$. Player p can make money selling credits to the market for pollutant c if their benefit curve is above the credit market curve. In contrast, Player p can save money purchasing credits of pollutant c if their benefit curve is below the credit market curve. For instance, Player 1 has an incentive to sell Q credits to the market, while Player 2 has an incentive to buy them. In general, the opposite relationship is true for N.

More subtly, Player 2 can make money selling N credits only when the BMP investment cost is lower than the credit price. This can be observed in the lower right hand frame of Figure 3.5. The credit market curve crosses the optimal investment curve in two places. Thus, some technologies are financially viable to generate profitable credits to the N market, while others are not. This contrasts with Player 1 for sediment (Q) where BMP investments are always profitable in this market regardless of cost.

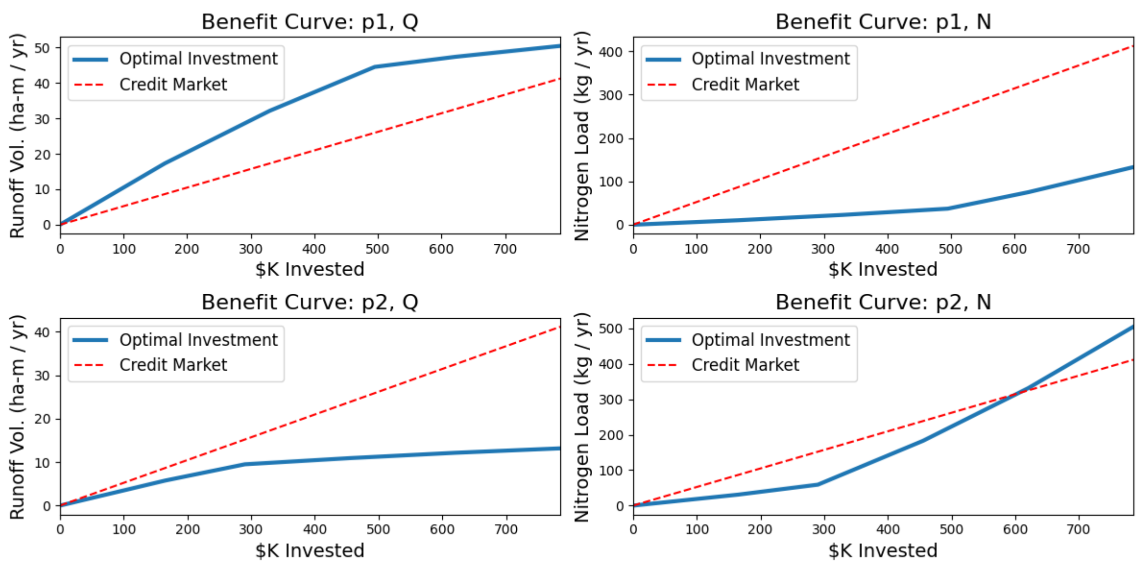


Figure 3.5: Visualization of trading insights

Player heterogeneity, visualized as the differences among benefit curves, can have implications for equity. Taken together, the KKT conditions and the market-clearing constraints imply that the players must share the cost burden equally for there to be an economic equilibrium in the credit-trading market. In mathematical terms, this means that π_c must equal $\gamma_{p,c}^{min}$ per (3.14b).

This equal cost burden could be unfair if environmental negligence drives the stormwater pollution. TMDL-C3 could represent such negligence using excessively high initial pollution loadings, $\hat{o}_{p,c}^{init}$. In such a case, a negligent player who pollutes more overall may be able to unfairly offload some of their regulatory burden to another player. This possibility should be considered in the evaluation of the viability of the credit market as it pertains to Challenge #1.

3.6.2 Analysis of Extreme Years

The stylized river basin demonstrates how a stochastic model can help analyze extreme years for pollution generation. In this context, an extreme year refers to an abnormally high level of pollution occurring in a given year. Understanding extreme years is important to assess risk to aquatic environments because continuous-exposure, toxicity tests do not generalize harm to aquatic organisms *in situ* [91]. Additionally, sediment, a major pollutant in urban watersheds like the Anacostia, is mostly delivered in extreme events [92]. By extension, average pollutant loadings can distort relevant information related to how extreme events cause harm to aquatic environments. Thus, TMDL-C3 provides more information to better address Challenge #3 than a non-stochastic model.

Figure 3.6 illustrates how an extreme year for pollution generation can be incorporated into TMDL-C3. The annual runoff summed across both players is plotted on the x axis, and the frequency of occurrence is plotted on the y axis. In this context, let the extreme year represent a pollution-loading scenario that crosses the threshold of harm to an aquatic environment. Additionally, let the stringent average refer to the average of a distribution that never crosses the extreme year threshold.

In the left-hand frame, the results for the stringent average constraint (S2) are shown, which does not explicitly consider the magnitude and frequency of the extreme year. To compensate for this, the BMP investment is very high such that the loading for the extreme year is never attained. Put another way, this is a conservative strategy for avoiding the extreme year. The reference watershed approach is a practical application of this strategy. This approach attempts to curb pollution such that the watershed mimics another unimpaired, reference watershed on average.

In the right-hand frame, the results for the extreme-event chance constraint (S3) are shown. Relative to the stringent average constraints in $S2$, these chance constraints reduce BMP costs significantly without much reliability loss (i.e., $\alpha_{p,c} = 0.9$). Additionally, the stringent average from the left-hand frame also remains only slightly under the mean for these results. This is possible because the uncertainty of pollution loadings is explicitly modeled with probability distributions instead of relying only on average values. The extreme year is also assumed to be known explicitly as $o_{p,c}^{allw}$.

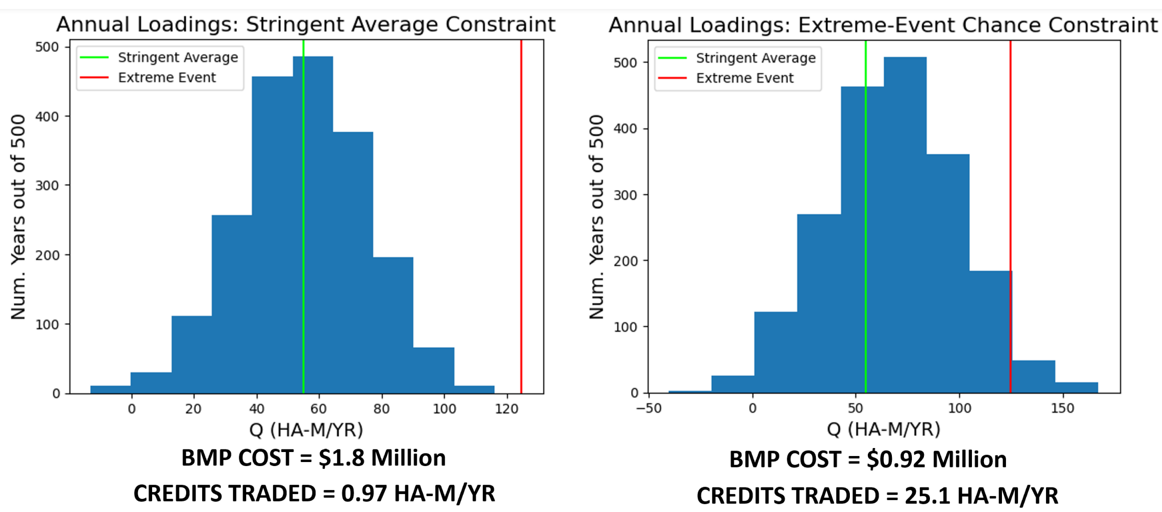


Figure 3.6: TMDL-C3 analysis for an extreme year

In this context, data uncertainty associated with Challenge #3 is a very important consideration because it is also interconnected with both Challenges #1 and #2. In terms of Challenge #1, the BMP installation cost to achieve the conservative distribution is nearly twice as expensive as the extreme year distribution ($1.8 Million vs. $0.92 Million). This difference in cost is largely related to the diminishing returns of implementing more BMPs. In terms of Challenge #2, there is also less trading potential because there are fewer ways to satisfy the TMDLs. The extreme year distribution has over 25 times the credits traded than the conservative distribution (25.1 ha-m/yr vs. 0.97 ha-m/yr).

3.7 Anacostia Case Study

The Anacostia River is a tributary to the Potomac River and the Chesapeake Bay. The river and its tributaries are located in Eastern Washington DC, Prince George's County, Maryland, and Montgomery County, Maryland with a combined stream channel length of nearly 300 miles (see Figure 3.7). The watershed is approximately 176 square miles in area with a population of more than 800,000 people. The aquatic habitat is home to 50 species of fish and 200 species of birds. Approximately 70% of the watershed is developed with 25% of the area consisting of impervious surfaces. Such a development pattern causes volatile flow in the tributaries and stagnant flow in the main branch [93].

The Anacostia Watershed is an instructive case study in TMDL implementation challenges. It is a moderate-sized watershed with multiple management jurisdictions (Challenge #2). These jurisdictions seek to base their continued cooperation on the most cost-effective pollution-reduction strategies (Challenge #1). Urban pollution has significantly hindered the river's ability to meet its designated use as fishable and swimmable. Furthermore, the pollutants are largely

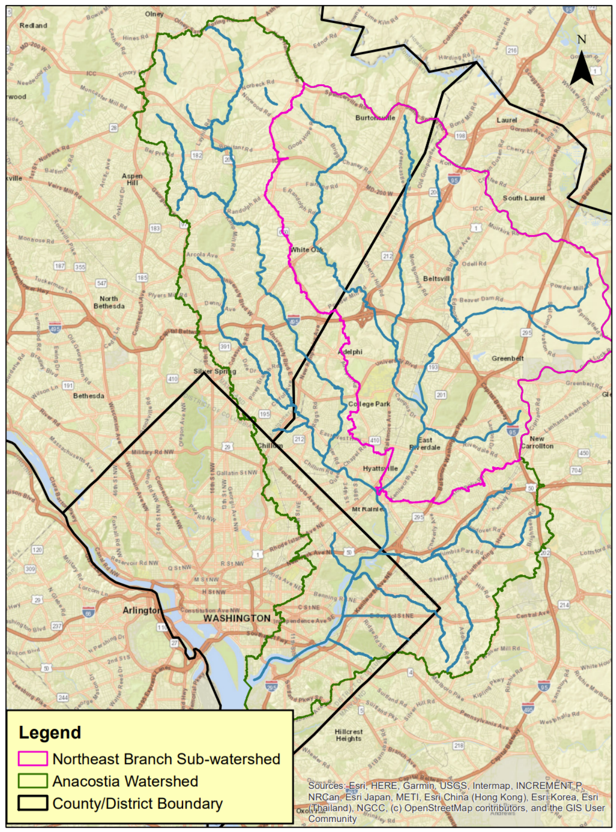


Figure 3.7: Anacostia Watershed and the Northeast Branch

delivered during extreme weather events. This creates data uncertainty (Challenge #3) in the form of pollutant-loading volatility. Considering these relevant issues, this watershed serves as a realistic case study for this chapter.

The pollution in the Anacostia has historically prevented the river from being appropriate for fishing and swimming. Runoff from impervious surfaces has contributed to excessive erosion and deposition of sediment. Sewage overflows have contributed fecal bacteria to the waterways. The improper disposal of trash has also been a problem. Additionally, legacy contaminants in the form of PCBs are present in the sediment due to historical industrial activity. To address these issues, TMDLs have been developed to guide the reduction of these pollutants [94] [95].

TMDL implementation in the Anacostia River basin also provides an opportunity to improve social equity and environmental justice. BMPs like rain gardens and green roofs can function as parks and green spaces, which promote physical, mental, and social health [96]. These health benefits are particularly relevant to Prince George's County, where systemic health inequities exist in non-white, low-income communities [97].

These TMDLs have been very difficult to implement because the Anacostia is one of the most urbanized sub-watersheds of the Chesapeake Bay. In urbanized settings, pollution is usually conveyed through stormwater systems with limited treatment options. For instance, the Anacostia nutrient TMDL calls for a 79% reduction of nitrogen loads. However, stormwater retrofits usually remove less than 70% of nitrogen [98]. This context helps to explain why, as of 2019, the Anacostia TMDLs were only implemented to 12%, 21%, and 9% for sediment, phosphorus, and nitrogen, respectively [99].

Despite the limited TMDL implementation progress, the associated water-quality improvements have caused a rebound of aquatic life in the river. The acreage of submerged aquatic vegetation (SAV) is a frequently cited metric because SAV serves as a habitat for many other aquatic species [100]. SAV was completely absent from the Anacostia River starting in 2003. However, it reappeared in 2013 and has been trending upward ever since [101].

The SAV population still remains highly vulnerable to short-term increases in sediment and nutrients. Higher concentrations of these pollutants diminish water clarity, which blocks sunlight from reaching SAV [90]. For example, SAV declined sharply in 2018 due to excess sediment from stream-bank erosion. This was also the wettest year on record for the DC region. Another SAV decline in 2021 was attributed to cloudy water during the growing season. Algal blooms from excess nutrients have also played a role in short-term water-clarity reductions [101].

Given this context, this Anacostia case study illustrates how TMDL-C3 could be used to help plan near-term BMP investments. These near-term recommendations support the long-term TMDL implementation goal in two important ways: First, they identify how existing BMP technologies can preserve the progress of rebounding aquatic ecosystems. Second, they provide learning opportunities to improve the effectiveness of BMP technologies and investments.

In terms of the first point, the chance constraints in TMDL-C3 relate BMP investments to extreme years for pollution generation. These extreme years can be chosen to correspond to a past disruption of a rebounding aquatic ecosystem. The 2018 loss of SAV is an example of such an extreme year. Thus, one would be interested in a BMP investment scheme that reduces the likelihood of such extreme pollution. In contrast, the sediment TMDL is based on a desired average annual loading [102], which is harder to relate to specific events.

In terms of the second point, improvements to BMP efficiencies and costs may make the Anacostia TMDLs easier to meet in the future than they are today. In this paradigm, learning from short-run experience enables technological solutions to become more attractive in the long run. There is some empirical support that these ideas apply at least in part to photo-voltaic solar energy [103]. Theoretical models have also been developed for how technological learning could apply to stormwater management [104] [105].

Learning from experience also applies to the TMDL itself. The Anacostia's Nutrient TMDL document says that the TMDL will be implemented in an "adaptive and iterative" process [106]. In such a scheme, BMPs will be put in place and their effectiveness will then be assessed through in-stream monitoring. This information will then be used to adjust the implementation strategy if necessary. This process, when repeated over time, is expected to approximate the TMDL goals more and more closely. This case study can be thought of as providing planning details for one such iteration.

With this background in mind, the Anacostia case study's research questions can be stated as: 1) How much progress can be made in TMDL implementation given current pollution mitigation technologies and the state of knowledge regarding the assimilative capacity of the Anacostia's aquatic environment? 2) How can the desired progress be translated into a plan for BMP installation throughout the watershed? 3) How might the municipal governments in the watershed coordinate their actions under this plan to achieve efficiencies?

The answers to these questions in the subsections that follow are intended to be illustrative. Policy recommendations arising from these research questions will require a broader scope and more recent data than considered in this chapter. However, the available data validates the feasibility of this chapter's technical approach, which is described next in Section 3.7.1.

3.7.1 Technical Approach

This case study focuses on the Northeast Branch (NEB) sub-watershed of the Anacostia River (Figure 3.7). The NEB sub-watershed includes portions of two Maryland counties: Montgomery (MC) and Prince George's (PG). The two county governments are modeled in TMDL-C3 as the primary decision-makers. This scope was chosen to make use of a pre-existing water-quality model of the NEB that was developed at the University of Maryland using the Hydrological Simulation Program Fortran (HSPF). This NEB water-quality model is based on a version of the Chesapeake Bay Watershed Model.

3.7.1.1 Water-Quality Model

HSPF is a lumped-parameter modeling environment [4], which simulates hydrologic and water-quality loadings from land segments and the transport, erosion, and deposition of sediment within streams. The model used in this study (NEBWQ) is based on Phase 5.3 of the Chesapeake Bay Watershed Model (CBWM5.3) [107].

Table 3.4 summarizes the land areas simulated in the NEBWQ by land use and county. Most broadly, HSPF subdivides land uses into pervious and impervious segments (PERLND and IMPLND modules). Pervious land includes forest, open land, and several types of urban land (i.e., residential, commercial, and institutional). Pervious urban land is likely to contain landscaping (e.g., lawns, mulch, etc.). This contrasts with forest, which is more likely to have natural vegetation and soils. The original CBWM5.3 simulated 21 pervious land uses and 3

[4]Lumped parameter means that watershed features such as land areas and stream reaches are modeled as discrete segments instead of continuous features. This eliminates the need to solve partial differential equations, which can be very computationally intensive.

impervious land uses for each county; this study simplified the land uses to 7 pervious and 2 impervious for each county; this study also introduced a distinction between residential land served by central sewer and by local septic systems. Land response is simulated on a per-unit-area basis; each unit response is multiplied by the corresponding land area. Water flows and pollutant delivery are combined in HSPF's reach/reservoir (RCHRES) module.

Table 3.4: Anacostia Northeast Branch land areas by usage

		Montgomery County		Prince George's County	
CODE	LAND USE	Hectares	%	Hectares	%
ic	impervious commercial	476	8.9%	1583	11.6%
ir	impervious residential	548	10.3%	864	6.3%
for	forest	1090	20.5%	4196	30.8%
opn	open land	422	7.9%	2498	18.3%
lrc	low-density residential on central sewer	428	8.1%	190	1.4%
hrc	high-density residential on central sewer	747	14.1%	1959	14.4%
lrd	low-density residential on decentralized septic	435	8.2%	192	1.4%
hrd	high-density residential on decentralized septic	747	14.1%	840	6.2%
pci	pervious commercial / institutional	423	8.0%	1296	9.5%
	TOTAL	5316	100 %	13618	100 %

Differences between the counties are important context for interpreting the model results from TMDL-C3. PG has more developed land than MC in the NEB. It has six times the amount of open land as MC (2498 vs. 422 hectares) and over 3 times as much impervious commercial land (1583 vs 476 hectares). By contrast, it only has roughly 1.5 times more pervious urban land (4477 vs. 2781 hectares).

The constituents modeled in this case study are sediment and nitrogen. The interplay of these constituents is important: reducing sediment without decreasing nutrients can lead to algae blooms. Considering this interplay, 80% reduction of nitrogen is required in the Anacostia TMDL to compensate for commensurate sediment reductions in the sediment TMDL [108] [106].

In urban streams, much of the sediment outflow is generated from stream bank erosion due to excess runoff from paved areas [73]. To avoid detailed process modeling, this study uses runoff (Q) as a surrogate for stream bank erosion [77]. This study denotes washoff sediment from land surfaces as S and total nitrogen as N. Other pollutants, such as bacteria and PCBs are not modeled because they already are being addressed within established projects [109] [110].

BMP investments are modeled as transformations from one land use to another less intensive one in terms of pollution generation. These transformations are summarized in Table 3.5. For instance, transforming impervious land to be hydrologically similar to open land is consistent with installation of pervious pavement because such a transformation would increase the infiltration rate without using vegetation. A similar logic applies to the other transformations in the table. Table 3.5's rows present the land-use transformations and the BMPs that they are assumed to represent in this case study.

This land-transformation scheme determines how the export coefficients are assigned. The starting land has an export coefficient $\hat{e}_{p,c,w,l}$, and the transformed land has a reduced export coefficient $\hat{r}_{p,c,t,w,l}$. The reduced export coefficient is equivalent to the export coefficient for the transformed land use. As an example, consider installing pervious pavement (PRVP) on impervious commercial land (IC). For a given p, c and w, $\hat{r}_{p,c,PRVP,w,IC} = \hat{e}_{p,c,w,OPN}$ where OPN refers to open land.

Table 3.5 also presents the assumed treatment fractions and marginal costs for these BMPs, consistent with the watershed modeled in the StormWISE paper [77]. Similar to the Anacostia, that watershed is in an urban area of the U.S. Mid-Atlantic region. Additionally, the costs used in that study, circa 2010, are from the same time frame that the Anacostia TMDL was approved. Thus, this case study assumes that the investment recommendations can be understood in retroactive terms. Comparing how current investments follow these recommendations is a potential area for future research.

Table 3.5: BMPs for the Northeast Branch sub-watershed of the Anacostia

Starting Land Use(s) (l)	Transformed Land Use	Interpretation (t)	$c_{t,l}^{site}(\$K/hectare)$	$f_{t,l}$
ic,ir	opn	pervious pavement (prvp)	907	0.25
ic	pci	impervious disconnection , commercial area (impd)	84	0.6
ir	hrc	impervious disconnection , residential area (impd)	84	0.6
ic,ir	for	on-site storage BMP mimicking pre-development conditions (pre)	1285	0.15
opn,lrc,hrc,pci	for	tree planting (plnt)	22	1
lrd,hrd	for	septic conversion and tree planting (plnt)	600	0.75
lrd	lrc	septic conversion only (sc)	578	0.25
hrd	hrc	septic conversion only (sc)	578	0.25

3.7.1.2 Pollutant Targets

The Anacostia's TMDL documents [102] [106] set forth the required loadings for sediment and nitrogen. Table 7 of the sediment TMDL [102] sets the loading target for the NEB to 3,814 tons/year. This means that at full TMDL implementation, the loadings of sediment are not expected to exceed this amount on average. The TMDL documents require nitrogen to be reduced by 80 % on average. Thus, for nitrogen, this study defines the target for full TMDL implementation to be $0.2\bar{o}_{p,N}^{init} \quad \forall p$.

Due to the challenges of achieving full TMDL implementation, the o^{allw} parameters are not assigned to these TMDL targets directly. Instead, the o^{allw} parameters are set to the flow and wash-off sediment loadings for Water Year (WY) 2021 [5]. These loadings were enough to cause SAV to die back during the growing season [101]. The SAV growing season is from April to October [102], which is mostly within the given water year. The investments made to reduce the frequency of exceeding the 2021 loadings are then related to fractional implementation of the TMDL targets.

[5] A water year is tracked from October 1st of the previous year to September 30th of the current year.

3.7.1.3 Modeling Strategy

The complexity of a real-world watershed requires a more sophisticated programming algorithm to parameterize TMDL-C3 than the stylized model of Section 3.6. This algorithm consists of NEBWQ, TMDL-C3, and an interface to manage the input and output between these two models. This interface, denoted the NEB Front End, is implemented in an interactive python (iPython) Jupyter Notebook [6]. Figure 3.8 presents a sequence diagram depicting how inputs and outputs are passed among the main algorithm modules.

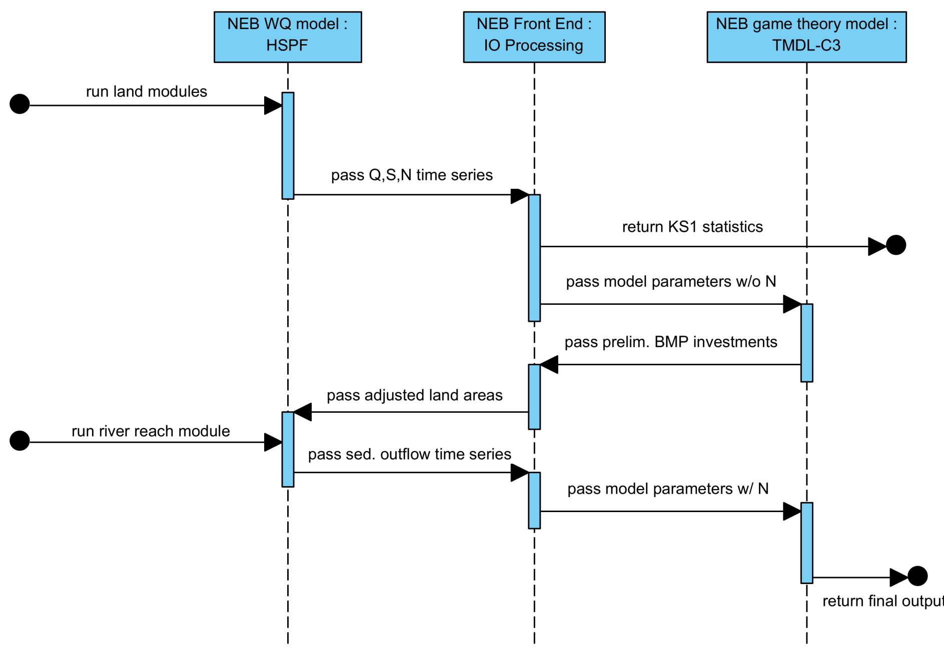


Figure 3.8: Algorithm sequence diagram for the Anacostia Case Study

This algorithm executes in four main phases. In Phase 1, NEBWQ runs. In Phase 2, TMDL-C3 runs to identify the preliminary investments to reduce the Q and S loadings for WY 2021. In Phase 3, the NEBWQ model runs again, translating these investments into progress towards the sediment TMDL. In Phase 4, TMDL-C3 runs a final time with load reduction re-

[6]The scripts in this Jupyter notebook were written by the lead author using open source python packages.

quirements for N. Between the phases, the NEB Front End receives input passed to it from one model (i.e., NEBWQ or TMDL-C3) and passes processed input to another.

In Phase 1, NEBWQ runs, passing daily time series of Q, S, and N from WY 1985 – 2004 to the NEB Front End. These represent estimates of the initial, untreated loadings from each land area. The NEB Front End sums these daily time series into annual time series. It then computes the sample means, variances, and covariances for the export coefficients and initial loadings from these annual values. The NEB Front End combines these summary statistics with the other model parameters (e.g., land areas, BMPs) without N and passes them to TMDL-C3.

The NEB Front End also returns the one-sample Kolmogorov–Smirnov (KS1) test statistics for each random model parameter. This test is done to check the normality assumptions that are discussed in Section 3.5.2. The null hypothesis (i.e., H_o) is that the random parameter is normally distributed. Each test reports the probability of the null hypothesis, $P\{H_o\}$. The results of these tests are analyzed and discussed in detail in Section 3.7.2.

In Phase 2, TMDL-C3 runs, determining preliminary BMP investments intended to reduce the annual exceedance probability of the Q and S loadings that were observed in WY 2021. This study uses WY 2004 as a surrogate for WY 2021 because 2021 is not included in the NEBWQ. The two years had similar annual discharge: 11,130 and 10,320 hectare-meters for 2021 and 2004, respectively [111]. The NEB Front End then passes adjusted land areas, based on these investments, to NEBWQ.

In Phase 3, NEBWQ runs again, passing a sediment outflow time series to the NEB Front End. The NEB Front end then calculates the average annual sediment outflow (i.e., X) obtained from the adjusted land areas. The NEB Front End calculates the percent TMDL as follows:

$$\%TMDL = \frac{5,231 - X}{5,231 - 3,814} \tag{3.17}$$

where 5,231 (tons/year) is the average initial sediment outflow in the NEB and 3,814 (tons/year) is the sediment loading target in the TMDL.

Finally, the NEB Front End calculates o^{allw} for nitrogen that corresponds to the same percentage of TMDL implementation. The model parameters with N are then passed back to TMDL-C3.

In Phase 4, TMDL-C3 runs for a final time. It includes the extreme year constraints from Phase 2 but also includes the o^{allw} constraints for N loading reduction. This is done to ensure that the final answer reflects roughly even progress between the sediment and nitrogen TMDLs.

3.7.1.4 Water-Quality Model Inputs

The inputs to the NEBWQ model consist of time series of weather-related data and atmospheric deposition of nitrogen, and parameters that represent the physical characteristics of each land segment. The weather-related time series include: 1. observed precipitation, 2. temperature, and 3. hourly potential evapotranspiration (PET) for MC and PG. PET represents the combined potential for water to evaporate directly from surface or soil or transpire through plants; actual transpiration rate varies according to seasonal changes in vegetative density and water availability. CBWM5.3 [107] provided the input data from Jan. 1, 1984 through Aug. 30, 2005 on an hourly basis. CBWM5.3 also provided monthly atmospheric deposition rates of three forms of nitrogen. Nitrogen input rates due to septic systems were estimated following [112]. Application of fertilizer was restricted to residential areas because agricultural land in the basin is negligible and mainly pasture; fertilizer application was simulated during the growing period, with rates estimated following [112].

Land segment parameters establish properties such as groundwater infiltration rates, vegetative cover, overland flow rate, sediment wash-off potential, and various nitrogen transformation rates. These parameters are assigned by land use. To represent BMP implementation, the NEBWQ model does not change land segment properties, but rather changes the area associated with each land use from run to run, as summarized in Table 3.5. That is, the export coefficients calculated for each land use type remain unchanged, while the area multiplying the coefficient is altered, adjusting the overall pollutant delivery volume.

3.7.2 Results

This section presents the results of the Anacostia Case Study. These results support two main lessons learned: (1) the normal distribution assumption generally holds well for the benefit slopes and the initial loadings, but there are some important exceptions. (2) The lack of BMP co-benefits between S and N drive the activity in the credit market. Like most urbanized watersheds, the reduction of runoff (Q) is important in the NEB. However, Q is traded freely in the credit market because many BMPs generate runoff reduction as a co-benefit. In contrast, wash-off sediment (S) and nitrogen (N) are not traded freely in the credit market because fewer BMPs have co-benefits for both S and N.

Figure 3.9 depicts a box plot of the 78 KS1 test results. The actual values are shown as points, which are spread out (i.e., jittered) along the x-axis to show the density of values. The

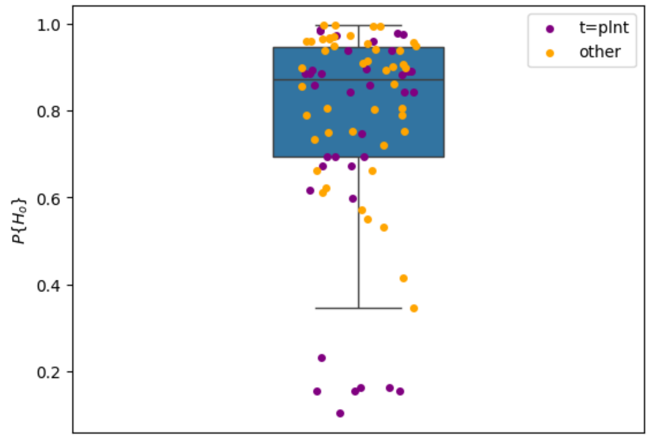


Figure 3.9: Boxplot with jitter showing the KS1 test results

purple color indicates the KS1 results involving benefit slopes for planting (plnt) BMPs. The orange color indicates KS1 test results for all the other random model parameters.

In general, the normal distribution assumption describes the random model parameters reasonably well. The median value of $P\{H_o\}$ is roughly 0.9, and many of the tests are clustered near or above this median. The inter-quartile range (IQR) is from roughly $P\{H_o\} = 0.7$ to $P\{H_o\} = 0.95$. Below the IQR, there exists an even distribution of KS1 test results from roughly $P\{H_o\} = 0.35$ upwards.

There are some outliers (i.e., $P\{H_o\} \leq 0.25$) where the normal distribution assumption is suspect. Within this set of outliers, $P\{H_o\}$ is as low as 10%. Interestingly, all of these outliers consist of benefit slopes for tree planting (plnt) investments. However, not all benefit slopes for plnt have low values for $P\{H_o\}$. Many of these benefit slopes are within the IQR.

Figure 3.10 depicts the normalized, empirical cumulative distribution functions (CDF) for the random parameters with the minimum, average, and maximum values for $P\{H_o\}$. The standard normal distribution is also plotted for comparison. As expected, the random parameters with the average and maximum values for $P\{H_o\}$ match rather closely to the standard normal distribution. In contrast, the random parameter with the minimum value of $P\{H_o\}$ does not match closely to the standard normal distribution. It's CDF is sparse near the extreme values.

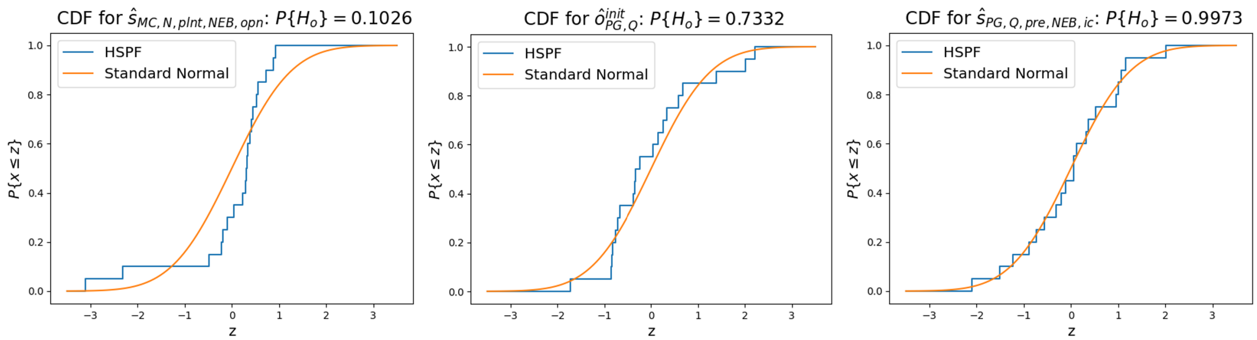


Figure 3.10: Normal distribution examples each with a sample size of 21 water years

Figure 3.11 summarizes the cost and reliability trade-offs from the output of the NEB Game Theory Model (TMDL-C3) and the aggregate optimization problem (Agg.) of Section 3.5.7. The exceedance probability of the sediment loading from 2021 decreases roughly linearly with the TMDL implementation percentage. In fact, at low % TMDL, the 2021 year is not extreme at all, it is expected to happen every other year. At just over 40 percent of the TMDL, the exceedance probability can be brought down to around 35 percent. The total implementation cost increases roughly linearly to get these benefits.

The solution pairs of TMDL-C3 and Agg. always have the same total investment cost but always differ in the cost distribution between the players. The analysis in Section 3.6 allows for the possibility of differences in cost distribution: the KKT conditions and the market-clearing constraints imply that the players must share the burden equally for there to be an economic equilibrium in the credit-trading market. One can thus interpret the market as providing the incentives needed for both players to invest in BMPs at the levels called for in the aggregate solution.

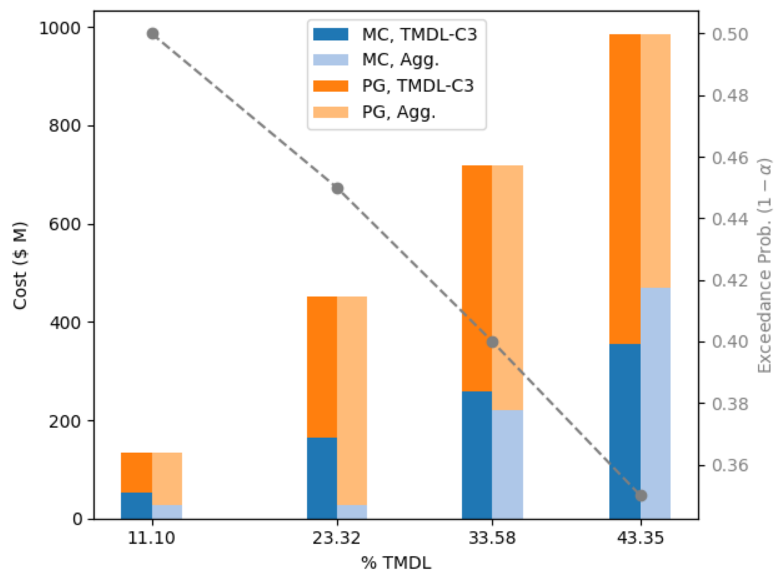


Figure 3.11: NEB Game Theory Model results summary

Figure 3.12 depicts a detailed breakdown of the BMP investments by player in TMDL-C3. Excluding the credit purchases, the BMP investments in the aggregate solution are identical to those shown in this figure. However, the credit purchases provide several insights into the total cost distribution between the players. Positive costs for credits are only present for S and N; the credit cost for Q is equal to zero. Most of the credit costs are associated with N. Furthermore, the player who purchases N credits always bears a higher cost in the TMDL-C3 solution relative to the aggregate one.

Figure 3.13 presents a parallel plot to explain why S and N have positive prices in the credit market. The correlation coefficients show that some BMPs are good at reducing flow along with S and flow along with N. However, there are few BMPs that are good at simultaneously reducing S and N. Specifically, open-land planting in PG (i.e., PG plnt NEB opn) is the only BMP with a non-negative correlation with N pollution reduction (approx. 0.2). In contrast, this same BMP has a correlation of 0.7 between Q and S. Additionally, the correlation between Q and N is always

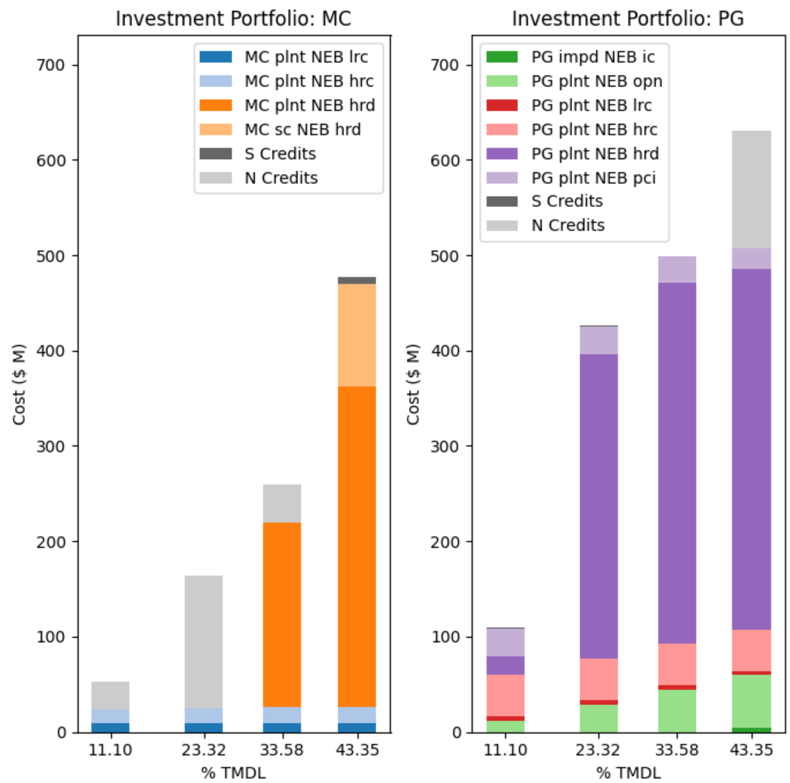


Figure 3.12: BMP investment portfolios by player

non-negative.

Figure 3.14 shows that the BMPs can roughly be divided into those that reduce S and those that reduce nitrogen. This provides some numerical specificity into the lack of correlation between S and N. Specifically, open-land planting in PG is the primary source of S reduction. For nitrogen, planting and septic conversion in residential land generates most of the benefits for nitrogen reduction. Of these, Figure 3.12 shows that high-density residential planting and septic conversion in both counties (i.e., 'MC plnt NEB hrd' & 'PG plnt NEB hrd') receives the most investment of all the BMPs.

Figure 3.14 also shows clear subsets of BMP investments as the percent TMDL increases. The investments indexed as 'MC plnt NEB lrc', 'MC plnt NEB hrc', 'PG plnt NEB hrc', and 'PG plnt NEB pci' appear in each solution while contributing roughly the same nitrogen reduction.

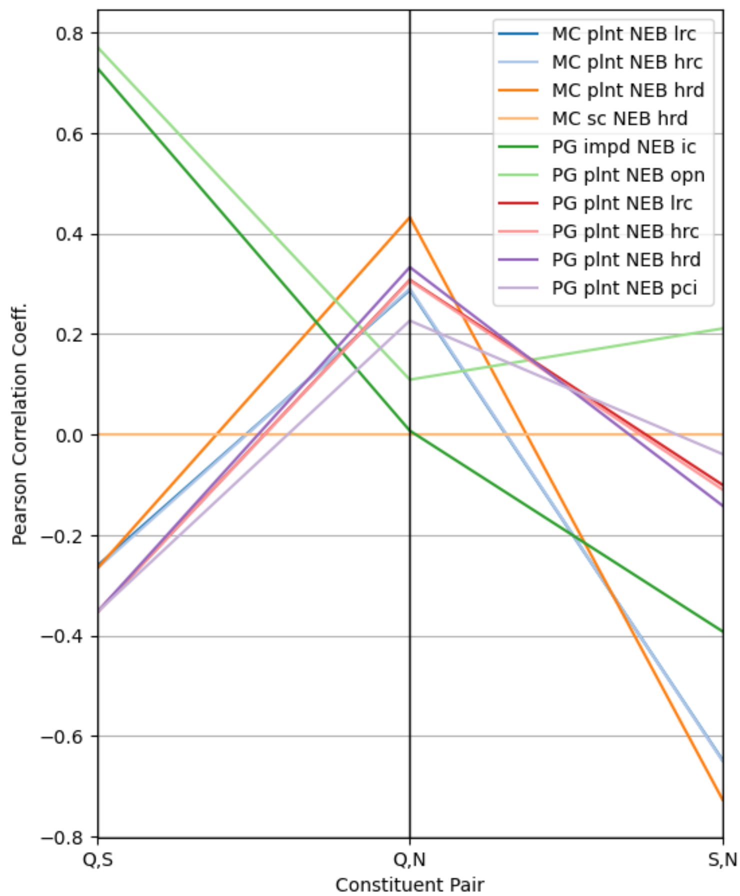


Figure 3.13: Constituent removal correlations by BMP

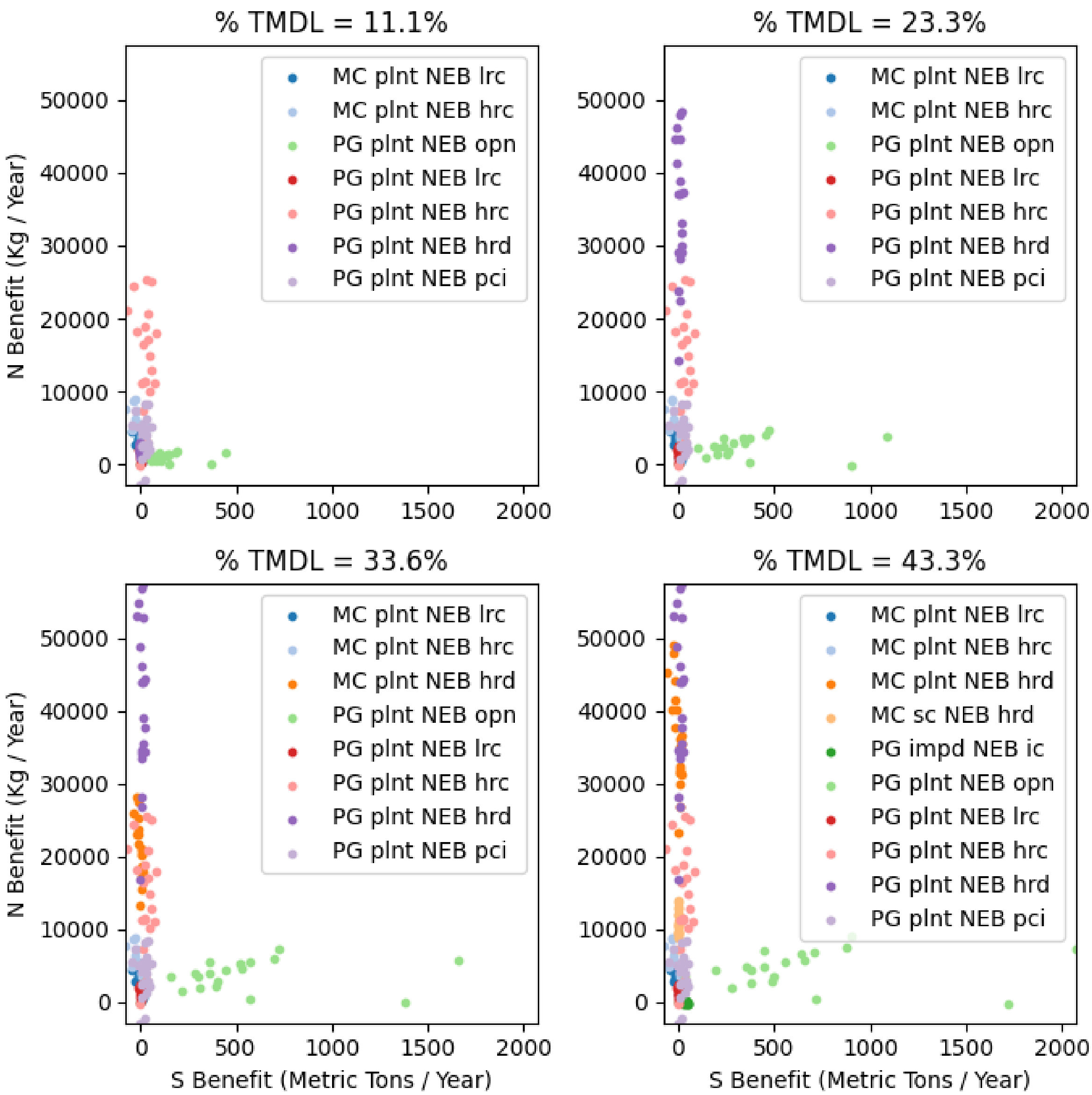


Figure 3.14: Detailed breakdown of BMP benefits

In contrast, other BMPs receive more investment as percent TMDL increases. These include the investments indexed as 'PG plnt NEB hrd', 'MC plnt NEB hrd' , and 'PG plnt NEB pci'.

Achieving full implementation of the sediment and nitrogen TMDLs will require the consideration of novel BMPs for nitrogen reduction. Several BMPs could receive more investment for sediment reduction such as impervious disconnection (impd) and mimicking pre-development conditions (pre). However, the BMPs that are good at nitrogen reduction are exhausted beyond 43 percent TMDL implementation. As mentioned previously, both the sediment and nitrogen TMDL need to be implemented simultaneously to improve water clarity for SAV growth.

With the nitrogen limits in mind, one can return to Figure 3.12 to understand the differences between each % TMDL run. In general, MC relies on credit purchases from PG for nitrogen. As % TMDL increases, PG also invests progressively more in planting in open land (i.e., 'PG plnt NEB opn'), which is good at sediment reduction (see Figure 3.14). This general trend holds true through 33.58 % TMDL.

However, at 43.35 % TMDL, the implementation scheme changes. PG exhausts its options for nitrogen reduction. To see this, PG's investments remain unchanged between % TMDL = 23.32 and % TMDL = 33.58 for everything but planting and impervious disconnection. Thus, MC increases tree planting ('MC plnt NEB hrd') and invests in septic conversion ('MC sc NEB hrd') while selling some of this investment as credits to PG. This is consistent with the land heterogeneity between the counties as discussed in Section 3.7.1.

3.8 Conclusion

The stylized model illustrates some of the conceptual issues associated with overcoming TMDL implementation challenges. The greedy heuristic is not optimal for project selection when there are pollution reduction co-benefits among alternative BMP choices. Additionally, player heterogeneity forms the basis for trading of constituents. Lastly, framing BMP investments in terms of exceedance probabilities reveals cost/benefit trade-offs that are difficult to observe with just average pollutant loadings.

The Anacostia model demonstrates some real-world insights for TMDL implementation. It shows that the progress towards a TMDL can be translated into an exceedance probability of a harmful loading scenario. Such an approach translates some of the uncertain hydrological data into probability distributions. Further, it emphasizes the challenges associated with implementing multiple TMDLs simultaneously. Specifically, choosing effective BMPs for nitrogen reduction limits the progress towards TMDL implementation. This limit also shows the role that the credit trading can play in nitrogen reduction.

Future research could incorporate other equity-related benefits into TMDL-C3. This could go beyond adding a constraint that caps BMP investment cost according to each player's ability to pay. For instance, a multi-objective approach could identify cost-effective BMP investments that prioritize social equity in TMDL implementation. To accomplish this, a series of constraints could be added that use BMPs as green space to reduce differential health outcomes in marginalized communities. For example, these constraints could relate BMP investments to improvements in air quality, physical activity, and mental health.

Chapter 4: Understanding the Role of Technological Complexity in Water-Resource Transitions using Stochastic, Bi-level Optimization

4.1 Introduction

Policymakers face a challenging dichotomy when establishing limits to the sustainable consumption of energy and other natural resources: consumption is derived from both accessible, limited resources and less accessible, but nearly unlimited resources (e.g., renewable energy, desalinated seawater). Harnessing the full abundance of the less-accessible resources depends on complex, technological solutions with uncertain, future prospects. Policies that are too optimistic regarding these technologies could fail to curb consumption enough, while pessimistic policies could curb consumption more than necessary.

Such technological trade-offs can be understood in terms of risk. The short-term depletion of limited natural resources can pay off if technology emerges to harness alternative resources in the long term. However, this short-term, resource-depletion policy carries the risk that the technology will not materialize. In such a case, economic decline, population decline, or both are possible undesirable outcomes.

Given this challenge, this chapter seeks to identify sustainable energy and natural resource policies that also account for technological transitions. This chapter concentrates on water-resource systems specifically to serve as a counterpoint to the already extensive literature on energy transitions [113]. However, this chapter's water model is also mathematically general to promote multi-disciplinary engagement among experts in energy and other natural-resource systems.

Technology plays an important role in water-resource systems because human engineering alters a natural environment's water quantity and quality. These technologies vary greatly in their complexity. A simple water-supply system for humans often features a shared well in a village. Simple technologies are typically used with freshwater sources such as streams, lakes, or groundwater. On the other hand, a complex water system often features reservoirs, water treatment facilities, and distribution networks of pipes and pumps. Even more complex technologies can also be used to treat seawater or wastewater.

Regardless of complexity, water-resource systems involve more than just their technical features. Socio-economic institutions construct and maintain these technologies. They also vary widely in complexity. Simple water institutions often rely on cultural norms for hygiene and resource sharing. Water utilities represent complex water institutions, which often have separate departments for planning, maintenance, construction, and finance. Other societal institutions, such as government and industry, are stakeholders who benefit from and influence the decisions of water institutions.

In most water-resource systems, societal norms, technologies, and economics have catered to the use of freshwater sources such as rivers, lakes, streams, and groundwater. Alternative water sources, such as seawater and wastewater, require a lot of energy and advanced technology to remove impurities and pathogens. These technologies are broadly viewed as either too expensive, risky, or unsanitary [114]. For example, desalination satisfies only 1% of global water demand

[115], and only 11 % of wastewater is reused [116].

Despite the dominance of freshwater sources, these alternative water sources play a central role in certain specialized contexts. Desalination has become commonplace in middle-eastern countries that have large oil reserves, few freshwater sources, and large coastal populations [117]. Additionally, recycling of wastewater into drinking water has become technically feasible and socially acceptable certain places such as Windhoek, Namibia. This became desirable because the city is located far from the ocean and has very scarce freshwater resources [7].

These alternative water sources are likely to become more relevant in more water-resource contexts in the future. Climate change is expected to alter the distribution of precipitation such that mega-droughts are likely in many regions across the world [118]. In contrast, seawater is highly abundant and thus is not vulnerable to changes in precipitation. Similarly, wastewater recycling allows small quantities of water to be reused multiple times, which effectively increases the water supply.

Water-resource issues are related to broader issues of sustainability. Resource extraction and pollution are human activities that impact the earth's natural systems including climate, ecology, freshwater, and nutrient cycles. These systems will likely destabilize unless resource extraction and pollution concentration limits are established at a global scale. These limits are collectively referred to as earth's system boundaries (ESBs). Research indicates that humanity has already crossed many of the ESBs including for surface water and groundwater [119].

ESBs are expected to place limits on economic growth because resource availability constrains industrial output. For instance, the index of industrial production (IIP) quantifies the gross output of the resource extraction, manufacturing, and energy sectors. A theoretical model of global population, food, resources, and pollution explores several scenarios for IIP change over time [120]. This model, supported by empirical data, suggests that IIP will peak in the mid-twentieth century due in part to resource depletion and pollution accumulation.

Complex green technologies (e.g., desalination and renewable energy) may help overcome the limits that ESBs (e.g., water supply and carbon concentrations) impose on industrial production. Put another way, industrial output can be decoupled from ESBs [121]. Indeed, technology often becomes more complex over time to overcome previous performance limitations. An allegorical example is the complexity of the modern jet engine. It evolved from the incremental additions of subsystems over time to regulate temperature, airflow, and combustion. These innovations accommodated progressively higher air pressures in airplane engines [122].

The allegorical jet engine example extends conceptually to environmental systems. Wastewater treatment technologies were developed to lessen the impacts of urban growth on water pollution [123]. Controls in the power and automotive sector reduced the emissions of non-methane, volatile organic compounds by half between 1990 and 2010 [124]. In both cases, environmental innovations introduced complexity in the form of new subsystems to water and air ESBs, respectively. These innovations helped to overcome the waste assimilation limits associated with human activity while allowing economic growth to continue.

Despite these historical arguments, unproven and complex green technologies will likely pose challenges. There is concern whether green technologies can be developed quickly enough to mitigate the ESB impacts [121]. For instance, existing desalination technologies bolster water supplies, reducing stress on the surface and groundwater ESBs. However, truly green desalination technologies need innovative solutions to reduce the discharge of saline waste products to the environment and to transition to renewable energy resources [125]. Otherwise, saline pollution and CO_2 emissions will continue to undermine the ecological and climate ESBs, respectively.

Consequentially, the decoupling concept has come under scrutiny in recent years. Alternatively, recent thinking asserts that the growth mindset of economic institutions is fundamentally incompatible with the ESB limits. In response, researchers have begun to envision how global society could thrive in the absence of economic growth. These alternative conceptions have been called "degrowth" mindsets. Degrowth generally emphasizes social change over technological change, including improvements to socio-economic equity and reduction of demand for natural resources [126] [127].

Regardless of one's opinion of degrowth or decoupling, transitions to technology, social norms, or both are required to re-stabilize the ESBs. Research into this imperative has become known as the field of sustainability transitions (ST) and has an impressive body of literature [128]. In ST, technology (e.g., desalination) and societal values (e.g., water-demand reduction) can change simultaneously. The next section presents a literature review of this field and explains how ST is used in this chapter to provide a novel ST modeling approach.

4.2 Literature Review

The ST field has many qualitative concepts that need more mathematical rigor [129]. Economists and complexity theorists have contributed some important mathematical details to ST related to innovation, economic growth, and the scale of cities [130] [131]. The field of operations research (OR) has contributed mathematical models to inform decisions regarding sustainable technology investment, infrastructure provision, and technology diffusion [132] [133]. As will be substantiated, this chapter is unique in that it integrates many of these modeling features together to support ST decisions related to energy and natural-resource allocation.

Economic theory plays an important role in ST because it addresses issues of economic growth, technology, and the price stability of scarce resources. Classical economic theory explains price stability, while subsequent economic theories link economic growth to technological innovation. Innovators of new technologies (e.g., personal computers) often disrupt the economic status quo and can capitalize on this disruption to gain an advantage over competitors [130]. Economic growth is possible in such a dynamic setting because market incentives favor technologies that progressively extract more value from commodities [134].

Classical economics often assumes diminishing returns, which means the marginal value of a resource diminishes with increasing utilization (i.e., negative feedback). This leads to the conditions for an economic equilibrium [135]. Equilibrium programming and game theory have been very successful in explaining how markets allocate scarce resources in sectors relevant to sustainability transitions such as energy [21] [82] [81] and water [24] [14]. These equilibrium models have been subsumed into mathematical programs with equilibrium constraints (MPECs) for infrastructure investment [20] and market regulation [25].

In contrast, technology can become more valuable the more it is utilized. This phenomenon is known as increasing returns to scale [130]. Firms that innovate early in a niche are more likely to increase the number of adopters of their technology relative to their competitors. The presence of adopters is likely to further adoption in a positive feedback loop [135]. For example, early electric vehicle (EV) manufacturers are more likely to have charging infrastructure and thus are more likely to continue capturing consumers.

Consequentially, an objectively inferior technology can become "locked in" because of early adoption [136]. This effect is called path dependence and is often associated with the difficulty of sustainability transitions with technological components (e.g., renewable energy).

For instance, non-renewable energy is likely to persist over renewable energy in places where fossil fuels are widely adopted for use in the power grid.

Statistical modeling plays an important role in ST because it can be used to examine the relationship between innovation, per-capita wealth, and city size. These relationships have been evaluated with the following power law model:

$$y = aN^b$$

where y represents a metric for wealth (e.g., GDP) or innovation (e.g., number of patents), N is population size, and a and b are the model's parameters. If $b > 1$, then the metric exhibits super-linear scaling with city population size. Similarly, if $b < 1$, then the scaling is sub-linear [131]. These scaling possibilities reveal the costs and benefits of cities with progressively larger populations.

The results from this power law model indicate that metrics for wealth and innovation exhibit super-linear scaling. Simultaneously, metrics for infrastructure (e.g., miles of utility lines, number of EV charging stations) exhibit sub-linear scaling. Many metrics for social and environmental problems (e.g., inequality, pollution) also exhibit super-linear scaling. Theoretical interpretations of these power law models [137] suggest that the social, environmental, and resource costs of city scaling will outpace wealth and innovation in the long run.

Two qualitative but important ST concepts have been synthesized from historical case studies [138] [128]. First, a regime is defined as the dominant technologies, standards, and institutional structures for a particular society (e.g., freshwater supply). To give another example, non-renewable power generation is a regime that is preserved by physical infrastructure, profit motive, and political incentives alike. Second, a niche is defined as a unique context where novel approaches can be developed independent of the dominant regime (e.g., Windhoek, Namibia for wastewater reuse).

Another qualitative idea in ST explains how regimes, like freshwater treatment and delivery systems, can persist even when they become ineffective. For instance, over-extraction of freshwater may continue even in extreme droughts. One approach to remedying such a situation is known as strategic niche management [139]. It seeks to transfer knowledge from a given niche and scale it up to redefine the capabilities of the regime. For instance, a desalination niche near the ocean could be scaled up to diversify freshwater supply regimes further inland.

The ST literature also calls for the use of several mathematical modeling frameworks to make these qualitative concepts more quantitative [129]. These frameworks include the following:

1. Mathematical models could clarify how sustainable technologies emerge and mature over time. Modeling these temporal aspects is called the *multi-phase* framework. For example, the US Military uses the technology readiness level (TRL) metric to track how a technology progresses from concept, to prototype, to final implementation. Research and development (R&D) activities enable such technological progress [140]. The probability of R&D success is often estimated using survey input from informed respondents such as subject-matter experts, project stakeholders, or both. One approach asks these respondents to assess several aspects of the R&D project of interest using an ordinal scale (e.g., 1,2,3,4) that includes qualitative evaluation criteria. For one of these ordinal scales, it is a best practice to assess technical complexity of the R&D project in this probability estimation

approach [141].

2. Mathematical models could clarify how infrastructure and new technologies evolve alongside one another (e.g., EVs and charging infrastructure). This modeling framework is called *co-evolution*.

3. *Social learning* could be modeled to characterize how agents learn from one another. For instance, how might a utility manager in a desalination niche transfer their knowledge to a utility manager in a freshwater supply regime who wants to augment their supply?

4. Lastly, mathematical models could clarify how niches fit within regimes, and how regimes fit into the surrounding landscape. For example, wastewater reuse innovations in Windhoek will not necessarily become commonplace elsewhere (e.g., surface water treatment regimes) unless the broader innovation landscape changes. Increased water scarcity due to climate change could be a potential driver for such changes. Modeling this nested structure is called the *multi-level* framework.

Recent works in OR model these ST frameworks and provide several insights. The models with multi-phase dynamics quantify the uncertainty inherent to the maturation of complex technologies. These models are either scenario-based [142] or probability-based, Markov Decision Processes (MDP) [132]. Models featuring co-evolution quantify infrastructure investment levels that support the emergence of new sewer designs [142] and electric vehicles [133]. Lastly, multi-level models explain how policymakers, companies (e.g., EV developers), and consumers interact [133].

Barring any unintentional omissions, no previous OR research integrates all four frameworks into a single mathematical model. For instance, the work that integrates the multi-level and co-evolution frameworks [133] lacks the temporal uncertainty of the multi-phase framework. However, the multi-phase models [142] [133] lack the multiple decision-makers in the multi-level framework. Furthermore, no OR work models either social learning or impacts to ESBs, such as the impact of withdrawals from surface water. These elements could provide ST with resource allocation insights and strategies to promote technology transfer (e.g., of desalination), respectively.

4.3 Contributions of this Chapter

This chapter integrates these four modeling frameworks into a single OR model enabling us to ask the following research question: **How does the uncertainty that is inherent to complex green technologies influence a policymaker's resource-allocation decisions?** Organized by framework, this chapter addresses this research question in the following ways:

1. The *multi-phase* framework is modeled using a two-stage, stochastic recourse problem [83]. In the first stage, research and development (R&D) is invested into a technology that offers the potential to unlock abundant resources (e.g., renewable energy, green desalination). In the second stage, the success of the R&D outcome is revealed.

2. Social norms for economic growth *co-evolve* with the success or failure of technology investment. This occurs because economic growth is coupled to resource availability, and resource availability is in turn dependent on the R&D outcome.

3. Different players have different R&D costs, but the investment of one player can lower the cost for others. For example, a desalination design for one region could be adapted for another at lower cost. This models *social learning*.

4. The *multi-level* framework is modeled using a bi-level optimization problem. This problem provides the main structure for resource allocation: Specifically, a policymaker oversees the management of an ESB, (e.g., climate, surface water, or ground water) and allocates a resource (e.g., allowance for carbon emissions, water volume) to lower-level consumers.

In Section 4.4, this chapter's mathematical formulation is presented. In Section 4.5, this formulation is applied to a stylized sustainability transition associated with water-resource management. This stylized example complements the already extensive literature on energy transitions [113]. It also builds on recent OR work in water systems where multiple decision-makers are explicitly modeled [143] [14] [15]. Lastly, Section 4.6 presents the final conclusions of this chapter.

4.4 Mathematical Formulation

This chapter builds on several sub-models to arrive at the final mathematical model of this chapter (Figure 4.1). Subsection 4.4.1 introduces the first sub-model, which introduces multiple phases for which population and economic growth change over time. Subsection 4.4.2 introduces the second sub-model, where technology co-evolves with population and economic growth. Subsection 4.4.3 introduces multiple decision-makers, which can learn from each other's technology investment decisions (i.e., social learning). Lastly, subsection 4.4.4 introduces the bi-level optimization problem to consider natural-resource allocation decisions.

The final, bi-level optimization model adheres to the following general form:

$$\max_{x} f(x, y)$$

s.t.

$$(x, y) \in Z$$

$$y \in S(x)$$

where x represents resource-allocation decisions and y represents how consumers decide to put these allocations to use. The objective function f is a social welfare metric, such as the consumer surplus of water or energy. The first three sub-models can be understood as developing Z and $S(x)$, which models how consumers arrive at their decisions (e.g., water or energy usage). This nested structure makes the bi-level optimization problem difficult to solve.

The terms defined in this section, which include sets, variables, and parameters, are summarized in Appendix C.4.1, C.4.2 and C.4.3 , respectively. The formatting conventions applied to these terms distinguish their type. Upper-case Roman letters represent model variables, while lower-case Roman letters indicate model parameters and endogenous cost functions. Probability parameters are one exception to this lower-case convention; they are identified using the $\mathbb{P}$ symbol. Lower-case λ and γ Greek letters represent Lagrange multipliers to their associated

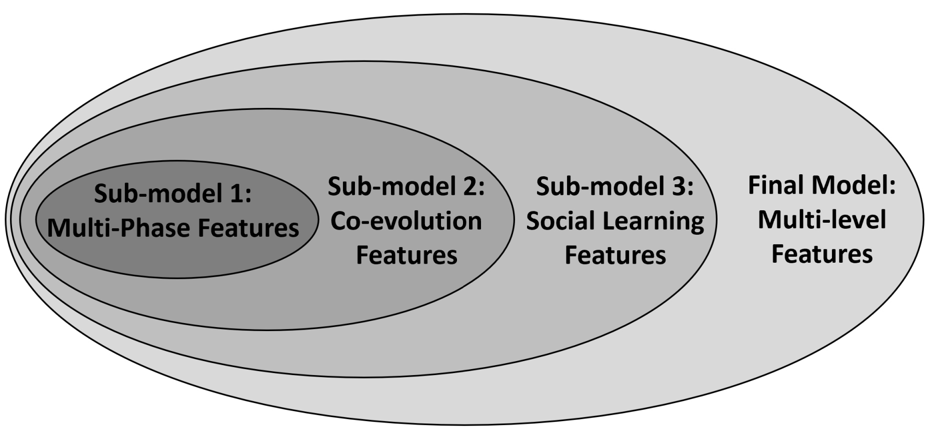


Figure 4.1: Organization of the mathematical formulation by ST modeling features

constraints. Superscripts distinguish similar terms (e.g., unit costs) from one another, while subscripts represent the indices of variables and parameters.

4.4.1 Multi-Phase Model Features

Each phase represents a discrete interval of time for which the players make or adjust their planning decisions. This interval is denoted as planning period t. The set of all such planning periods is denoted as $\mathcal{T}$. Realistically, the players have a limited planning horizon, so $\mathcal{T}$ is a finite set. For example, the planning horizon could be 30 years and there could be six planning periods of 5 years each within this horizon. In such a case $|\mathcal{T}| = 6$.

Variables that represent rates (e.g., flow of water, power per unit time) take on representative average values within each planning period. This is done to make the model easier to interpret, without loss of generality. For instance, the amount of water that flows into a region over a five-year planning period would be large. Instead, monthly averages are assumed because this is a representative timescale for resource consumption (e.g., utility billing of energy or water).

Consider an urban or rural development region that is managed by player $p \in \mathcal{P}$, which could represent a municipal government. At a discrete time period t in planning horizon $\mathcal{T}$, player p's region has a population $N_{p,t}$. Assume that each player derives a benefit b_p (e.g., tax revenues) for each member of the population. This population requires the consumption of a finite resource, $F_{p,t}$, which carries a cost c_p^f per unit. Lastly, emigration from the region, $E_{p,t}$, is possible, which carries a cost per capita of c_p^e. This emigration cost represents the lost economies of scale from maintaining infrastructure such as roads and utilities that were designed for a larger population. For example, Detroit, Michigan, USA lost 25% of its population between 2000 and 2010 resulting in declining city services, higher infrastructure costs, and greater social inequality [144].

Considering these population-dependent benefits and costs, each player maximizes the net discounted benefit for its region as follows:

$$\max b_p N_{p,1} - c_p^f F_{p,1} - c_p^e E_{p,1} + \sum_{2 \leq t \leq |\mathcal{T}|} d_{p,t}(b_p N_{p,t} - c_p^f F_{p,t} - c_p^e E_{p,t}) \tag{4.1a}$$

where $d_{p,t}$ is development region p's discount rate for planning period t.

This objective function is subject to the constraints of population growth. Other authors have modeled population growth in terms of a stochastic process [145] or super-linear scaling [131]. However, this chapter takes a simpler approach to population growth. Specifically, this chapter assumes that an individual in $N_{p,t}$ nets on average g_p additional individuals via reproduction or invitation to the region during each time period t. The population thus grows exponentially from a starting population n_p^i via the difference equation $N_{p,t+1} = g_p N_{p,t}$.

Unless resources are unlimited, exponential growth is not possible indefinitely. Thus, player p may need to cap the accommodations made for future population growth. Although this capping mechanism is not explicitly modeled, it could represent the reduction of land zoned for new residents. This chapter assumes that prospective residents above this cap will locate elsewhere instead. Thus, (4.1b) modifies the difference equation in the previous paragraph reflects the possibility of population caps:

$$N_{p,t+1} \leq g_p N_{p,t} \quad \forall t \in \mathcal{T} \tag{4.1b}$$

The population cap could be less than the current population if insufficient resources exist to sustain it. Such a case implies emigration, $E_{p,t}$, out of the region. The possibility of population loss can be expressed mathematically for both the first time period as well as subsequent time periods as follows:

$$N_{p,1} = n_p^i - E_{p,1} \tag{4.1c}$$

$$N_{p,t+1} \geq N_{p,t} - E_{p,t} \quad , \quad 1 < t < |\mathcal{T}| \tag{4.1d}$$

where n_p^i is the starting population and i indicates initial. As previously stated, emigration is assumed to carry a unit cost of c_p^e. This represents costs associated with maintaining infrastructure for a developed area with a previously larger population.

The population for player p demands a quantity q_p of resources (e.g., water) per capita. Supply of this finite resource $F_{p,t}$ (e.g., via groundwater), must be greater than or equal to the quantity demanded by the current population:

$$F_{p,t} \geq q_p N_{p,t} \quad \forall t \in \mathcal{T} \tag{4.1e}$$

Empirical research has validated the linear relationship of (4.1e) between resource consumption and population levels for both household electrical and water consumption [131].

The resource limit l constrains the supply of $F_{p,t}$ unless a withdrawal $W_{p,t}$ is made from a depletable reserve at time t. This limit is associated with an ESB (e.g., air, water, land, etc.). For instance, l could represent the amount of groundwater recharged by rainfall, while W could represent the over-extraction of groundwater reserves. For simplicity, this chapter assumes that withdrawal from the reserve does not incur any additional unit costs beyond c^f. Mathematically, this constraint on supply is as follows:

$$F_{p,t} \leq l + W_{p,t} \quad \forall t \in \mathcal{T} \tag{4.1f}$$

Withdrawals can continue up to the maximum accumulated amount of the depletable reserve. The accumulation available for withdrawal at time t is denoted as A_t. The maximum level of A_t is given as a^i, in time period 1 where the i superscript indicates initial. This chapter does not account for recharging the reserve (e.g., groundwater replenishment) or withdrawal losses. Mathematically, withdrawals are modeled as follows:

$$A_1 = a^i \tag{4.1g}$$

$$A_{t+1} = A_t - W_{p,t} \quad , \quad 1 < t < |\mathcal{T}| \tag{4.1h}$$

This emphasis on a depletable reserve, A_t, represents an important distinction between sustainability transitions and technology transitions in general. Specifically, the stored resource could be available in the current time period but is not replenished if depleted. Thus, long-term economic growth is not possible without the sustainability transition. More generally, technology transitions may be a prerequisite for any economic growth to occur. In such cases, careful management of depletable resources may not be an important consideration.

Sub-model 4.1 establishes the multi-phase features with the dynamics of population growth and resource constraints (assuming variable non-negativity). Figure 4.2 represents two potential solutions for a single player p. These solutions have many qualitative similarities to the familiar logistic growth curve [146] with two different paths to the carrying capacity. In both solutions, the benefit b_p is an order of magnitude larger than the cost c_p^f. The parameter $q_p = 1$ for simplicity, and the parameter $g_p = 2$. The entire input data is provided in Appendix C.1.

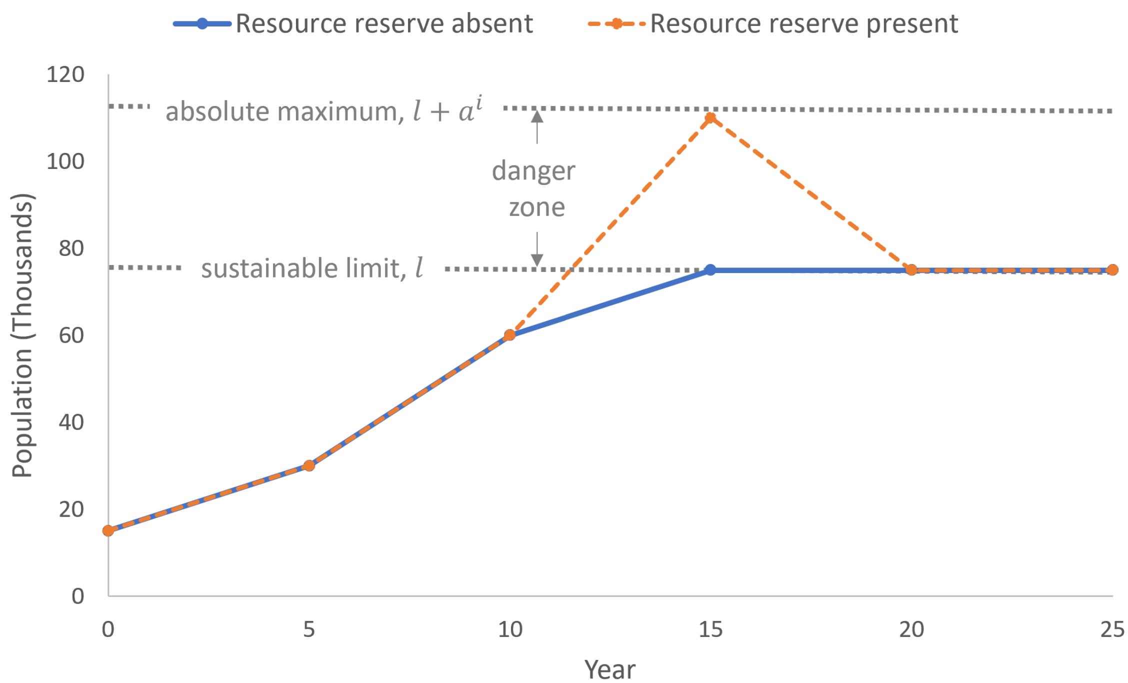


Figure 4.2: Illustration of temporal aspects

For both solutions, the returns to the resource (e.g., water) depend on the time interval with respect to the horizontal axis in Figure 4.2. The returns increase during years 0 - 10 as reflected in the growing population. Beyond this interval, the growth cannot be sustained: the population growth rate decreases due to l. For this reason, l is referred to as the sustainable limit. Similarly, consumption that exceeds l is called the danger zone in Sub-model 4.1.

As shown in Figure 4.2, the solutions approach l from either above or below. For one solution, the resource reserve is absent (i.e., $a^i = 0$), and the population approaches l from below because l cannot be exceeded. For the other solution, a resource reserve is present, and l is approached from above. The population overshoots l between years 10 and 15 and then declines back down to l between years 15 and 20.

The resource reserve and the discount rate account for this population overshoot and subsequent decline. The resource reserve of $a^i = 35$ units (e.g., $10^5 m^3$ water) is completely depleted between years 10 – 15 allowing the population to grow to 110 K. Between years 15 – 20, emigration occurs (i.e., $E_{p,20} = 35K$) because only l units of resources are now available. The associated emigration cost is discounted highly compared to the nearer term population growth because a discount rate of 10 % per year is assumed.

In either case, increasing returns would continue if l was larger. Overcoming the limits of l is consistent with technological innovation that taps into an alternative, potentially unlimited, resource (e.g., desalination of seawater). Thus, the phases of technological innovation can be understood in reference to l. The possibility of technological innovation is incorporated in the next subsection.

4.4.2 Co-Evolution Model Features

Now, suppose that each developer p can invest c_p^{RD} dollars into research and development for such a technology (e.g., desalination). Due to the complexity of such technologies, the return on this R&D investment (ROI) is uncertain. Thus, a discrete scenario $s \in S$ represents one of multiple ROI outcomes, which carries a probability $\mathbb{P}_p(s)$. Each ROI is the technology's cost as a function of the quantity of the practically unlimited resource, $c_{p,s}^u(U_{p,s})$. For example, $U_{p,s}$ could represent the quantity of water desalinated while $c_{p,s}^u(U_{p,s})$ is the corresponding cost.

The R&D investment, c_p^{RD}, is assumed to be a fixed cost that is either forgone or paid according to the binary decision $X_p^{RD} \in \{0, 1\}$, respectively. For instance, this fixed cost could represent the cost to install a pilot wastewater reuse plant or a renewable-energy-powered desalination facility. Future research could make this R&D cost continuous where larger investments translate into a high success probability $\mathbb{P}_p(s)$. Such decision-dependent probabilities are an example of endogenous uncertainty [147], which is a computationally challenging, emerging area of research.

The underlying probabilities $\mathbb{P}_p(s)$ of the scenarios are Bayesian in the sense that they are based on beliefs towards the technology. Subject matter experts are typically used to estimate the probability of a technology being successful. However, these probability estimates are still useful because they help decision-makers to hedge their technology investment decisions. Intuitively, this chapter assumes that these probabilities are related to the complexity of the technology.

This ROI uncertainty inhibits a decision-maker from knowing future events with certainty. In Sub-model 4.1, the decision-makers are assumed to have perfect foresight. Now, the decision-maker can consider only the current time period and the ROI scenarios for the next time period. Decisions made in the current time period are called first-stage decisions, while follow-up decisions are called second-stage decisions. For these reasons, Sub-model 4.2 is a type of two-stage, stochastic optimization problem [83].

Sub-model 4.2 is formulated to consider multiple two-stage problems in sequence. This enables decisions to be made over the whole planning horizon, as in Sub-model 4.1. Information from solutions in previous time periods (e.g., population levels) are provided as starting data for the current time period. The starting time period is called the "roll" (analogous to dice roll) and the collection of all such rolls is called the "rolling horizon." This rolling horizon approach reflects how decision-makers refine their decisions with the best available information at the time [80].

The variables $N_{p,t}$,$F_{p,t}$, and $E_{p,t}$ from Sub-model 4.1 are modified to conform with this rolling horizon approach. Notationally, assume that the current roll r occurs at time period t. For the variable $N_{p,t}$, the first-stage population term is $N^{FS}_{p,r}$, where r is a shorthand for $t = r$. Similarly, $N^{SS}_{p,r+1,s}$ reflects the second-stage population in time period $t = r + 1$ for a given scenario $s \in S$. For example, a scenario s could indicate desalination technology increasing in cost effectiveness. The same adjustments are also made to the variables $F_{p,t}$ and $E_{p,t}$.

The objective function (4.2a) seeks to maximize the expected payoff of R&D using this rolling-horizon approach. Specifically, the payoff is the net benefit of the first-stage decisions plus the discounted, expected net benefit of the second-stage decisions. The first-stage variables include the analogous terms to Sub-model 4.1 as well as the binary R&D investment decision, X^{RD}_p. Similarly, the second-stage also includes analogous Sub-model 4.1 decisions as well as the cost of the new technology $c^u_{p,s}$. As will be shown, this technology cost function is piecewise linear.

$$\max b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p \\ + d_{p,r+1} \sum_{s \in S} \mathbb{P}_p(s) \left(b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s}) \right) \quad (4.2a)$$

Objective function (4.2a) is not realistic on its own because it does not explicitly weigh the risk of undesirable R&D scenarios. Avoiding risk has value for many decision-makers even if taking risks also has benefits. In this chapter's context, planning for the benefits of green technology carries risk because the realized R&D scenario could fail to be economically viable. In such a scenario, the decision-maker could overestimate resource availability and lack enough to cost-effectively maintain a locality's population.

An improved objective function to address risk is developed presently. This objective function will use a weighted sum of the expected payoff in (4.2a) and a convex risk measure. The significance of convexity to the model in this chapter is explained further in Section 4.4.3. From this point onwards, player p's weight for risk is a parameter denoted as $\beta_p \in [0, 1]$. Naturally, the weight for player p's payoff is $(1 - \beta_p)$.

The primary convex risk measure in the stochastic programming literature is known as Conditional Value at Risk (CVaR). For player p, CVaR is the expected value of the net-benefit shortfall, $V_{p,s}$ [148]. A given scenario's net benefit is shortfall if it is smaller than the (1 - α_p)-quantile of the net-benefit distribution. The term $\alpha_p \in [0, 1]$ is an arbitrary model parameter. To calculate CVaR, an auxiliary decision variable, Z_p, is also needed.

CVaR is incorporated into Sub-Model 4.4.2 in Expression (4.2b), which is the improved objective function to expand upon (4.2a). Specifically, CVaR includes the terms in parentheses that are multiplied by β_p. As will be shown, additional constraints are implemented to calculate Z_p and $V_{p,s} \forall s$ in terms of model-specific benefits and costs (e.g., $b_p N^{SS}_{p,r+1,s}$, $c^u_{p,s}$). The optimal value of the auxiliary variable, Z^*_p, is the net benefit of the (1 - α_p)-quantile as long as this quantile is finite [149]. The remaining terms in this objective function include the payoff from (4.2a) times the weighting term $(1 - \beta_p)$.

$$\max \sum_{p \in P} \Big(1 - \beta_p\Big) \Big(b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p + d_{p,r+1} \sum_{s \in S} \mathbb{P}_p(s) \Big($$

$$b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s})\Big)\Big) + \beta_p \left(Z_p - \frac{1}{1 - \alpha_p} \sum_{s \in S} \mathbb{P}_p(s) V_{p,s} \right) \quad (4.2b)$$

Constraint (4.2c) calculates the net benefit shortfall, $V_{p,s}$, for each scenario s. At optimality, this is the $(1-\alpha_p)$ quantile payoff, Z_p^*, minus the optimal payoff in a given scenario. The payoff for a given scenario is simply (4.2a) without taking the expected value across all the scenarios. $V_{p,s}$ is also constrained to be non-negative for all scenarios s. Further, the $V_{p,s}$ variables are minimized in (4.2b). Therefore, $V_{p,s}$ is intuitively zero whenever a scenario's payoff is greater than Z_p^*.

$$
\begin{aligned}
&Z_p - \Big(b_p N_{p,r}^{FS} - c_p^f F_{p,r}^{FS} - c_p^e E_{p,r}^{FS} - c_p^{RD} X_p^{RD} + \\
&\quad d_{p,r+1}\Big(b_p N_{p,r+1,s}^{SS} - c_p^f F_{p,r+1,s}^{SS} - c_p^e E_{p,r+1,s}^{SS} - c_{p,s}^u (U_{p,s})\Big)\Big) \leq V_{p,s} \quad (\gamma_{p,s}^{rsk}) \quad \forall s \in S
\end{aligned}
\tag{4.2c}
$$

Expressions (4.2d) - (4.2o) re-express the constraints from Sub-Model 4.1 in terms of the rolling-horizon approach. These constraints appear more numerous compared to Sub-Model 4.1 before because they are explicitly defined for both the first and second stages instead of implicitly over all time periods. Importantly, the second stage constraint for supply exceeding demand, i.e., (4.2e), now augments the finite resource $F_{p,r+1,s}^{SS}$ with the practically unlimited resource $U_{p,s}$.

$$
F_{p,r}^{FS} \geq q_p N_{p,r}^{FS} \quad (\gamma_{p,r}^{dem1}) \tag{4.2d}
$$

$$
F_{p,r+1,s}^{SS} + U_{p,s} \geq q_p N_{p,r+1,s}^{SS} \quad (\gamma_{p,r+1,s}^{dem2}) \quad \forall s \in S \tag{4.2e}
$$

$$
F_{p,r}^{FS} \leq l + W_{p,t}^{FS} \quad (\gamma_{p,r}^{lim1}) \tag{4.2f}
$$

$$F^{SS}_{p,r+1,s} \leq l + W^{SS}_{p,t+1,s} \quad (\gamma^{lim2}_{p,r+1}) \quad \forall s \in S \tag{4.2g}$$

$$N^{FS}_{p,r} \leq g_p n^i_p \quad (\gamma^{max1}_{p,r}) \tag{4.2h}$$

$$N^{SS}_{p,r+1,s} \leq g_p N^{FS}_{p,r} \quad (\gamma^{max2}_{p,r+1,s}) \quad \forall s \in S \tag{4.2i}$$

$$N^{FS}_{p,r} \geq n^i_p - E^{FS}_{p,r} \quad (\gamma^{min1}_{p,r}) \tag{4.2j}$$

$$N^{SS}_{p,r+1,s} \geq N^{FS}_{p,r} - E^{SS}_{p,r+1,s} \quad (\gamma^{min2}_{p,r+1,s}) \quad \forall s \in S \tag{4.2k}$$

$$A_{p,r+1} = a^i - W^{FS}_{p,r} \quad (\lambda^{acc}_{p,r}) \tag{4.2l}$$

$$W^{SS}_{p,r+1} \leq A_{p,r+1} \quad (\gamma^{acc}_{p,r}) \tag{4.2m}$$

$$N^{FS}_{p,t}, E^{FS}_{p,t}, F^{FS}_{p,t}, W^{FS}_{p,t}, W^{SS}_{p,t+1} \geq 0 \quad , \quad t = r \tag{4.2n}$$

$$N^{SS}_{p,t,s}, E^{SS}_{p,t,s}, F^{SS}_{p,t,s}, U_{p,s} \geq 0 \quad \forall s \in S \quad , \quad t = r + 1 \tag{4.2o}$$

Sub-model 4.2 is non-linear due to the binary variable X^{RD}_p and the assumed piecewise structure of $c^u_{p,s}$. As will be shown, these non-linear terms make Sub-model 4.2 a mixed-integer linear program (MIP). The terms in parentheses next to the linear constraints represent shadow prices. These prices are only valid for true linear programs. However, in Section 4.4.3 onwards, the integer variables are either treated endogenously or represent the decisions of an upper-level policymaker. Therefore, these shadow prices are valid in the subsequent sections.

Additional constraints are needed to define the cost function c^u_p and its argument $U_{p,s}$. Specifically, the piecewise segments of c^u_p are assumed to be concave and increasing. This reflects an intuitive assumption of endogenous technological learning: the marginal cost of technologies often decreases with increasing utilization. Thus, the derivative of the total cost decreases as $U_{p,s}$ increases. Alternative conceptions of technological learning [103] are left for future research. This chapter assumes that U is implemented in $t = r + 1$. For notational simplicity, the time index is dropped (i.e., $U_{p,s,r+1} \equiv U_{p,s}$).

A combination of linear and binary variables are used to activate the piecewise segments [45] of c^u_p. These are modeled as two-segment functions (Figure 4.3). The three break-points are denoted as A, B, and C. The domain values at these break-points are 0, i^B_p, and i^C_p, respectively, while the function values are c^A_p, $c^B_{p,s}$, and $c^C_{p,s}$, respectively. The weighting terms $Y^A_{p,s}$, $Y^B_{p,s}$, $Y^C_{p,s} \in [0, 1]$ quantify how close the domain value $U_{p,s}$ is to the corresponding break-point.

Figure 4.3 also depicts these piecewise curves in terms of the ROI for each scenario $s \in S$. In the technological-improvement scenario (i.e., $s = 1$), the marginal cost decreases with increasing utilization consistent with technological learning. The technology reaches maturity between i^B_p and i^C_p with a marginal cost of $c^m_{p,1}$. In the technology-stagnation scenario (i.e., $s = 2$), the difference between c^A_p and $c^B_{p,s}$ in $s = 2$ is much greater than for $s = 1$. In this case, the marginal cost does not decrease.

Mathematically, (4.2p) - (4.2y) model these piecewise aspects to complete Sub-model 4.2. Expressions (4.2p) and (4.2q) model the function $c^u_{p,s}$ and its argument $U_{p,s}$, respectively. These expressions are defined in terms of the breakpoints A, B, C and the weighting terms between each breakpoint. Expressions (4.2r) - (4.2w) control the activation of each piecewise segment. In these expressions, the binary terms $X^A_{p,s}$ and $X^B_{p,s}$ activate the piecewise segments between A and B and B and C, respectively [45].

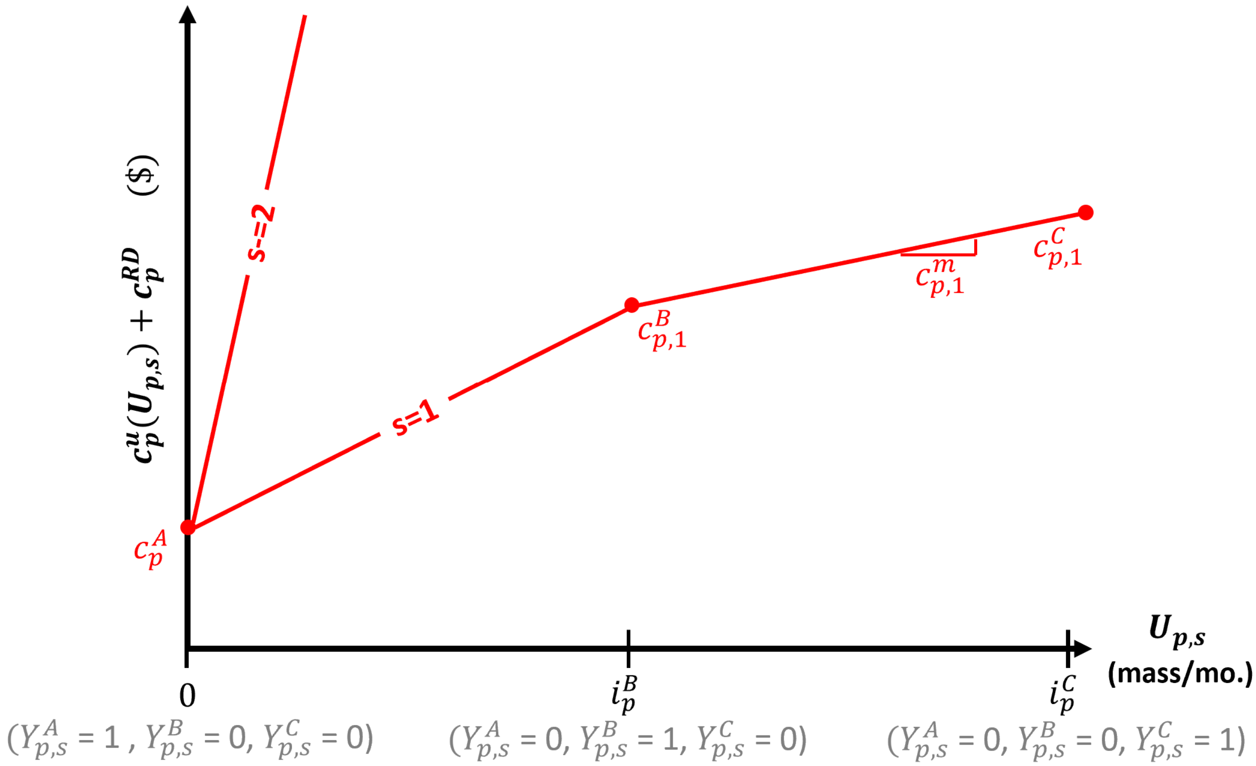


Figure 4.3: Technology cost curve details

$$c_{p,s}^u(U_{p,s}) = c_p^A Y_{p,s}^A + c_{p,s}^B Y_{p,s}^B + c_{p,s}^C Y_{p,s}^C - c_p^{RD} X_p^{RD} \quad (\lambda_{p,s}^{pw}) \quad \forall s \in S \tag{4.2p}$$

$$U_{p,s} = i_p^A Y_{p,s}^A + i_p^B Y_{p,s}^B + i_p^C Y_{p,s}^C \quad (\lambda_{p,s}^u) \quad \forall s \in S \tag{4.2q}$$

$$Y_{p,s}^A \leq X_{p,s}^A \quad (\gamma_{p,s}^A) \quad \forall s \in S \tag{4.2r}$$

$$Y_{p,s}^B \leq X_{p,s}^A + X_{p,s}^B \quad (\gamma_{p,s}^B) \quad \forall s \in S \tag{4.2s}$$

$$Y_{p,s}^C \leq X_{p,s}^B \quad (\lambda_{p,s}^C) \quad \forall s \in S \tag{4.2t}$$

$$Y_{p,s}^A + Y_{p,s}^B + Y_{p,s}^C = X_p^{RD} \quad (\lambda_{p,s}^{rd}) \quad \forall s \in S \tag{4.2u}$$

$$X_p^{RD} \in \{0, 1\} \tag{4.2v}$$

$$X_p^A, X_p^B \in \{0,1\} \quad , \quad X_{p,s}^A + X_{p,s}^B = X_p^{RD} \quad \forall s \in S \tag{4.2w}$$

$$V_{p,s}, Y_{p,s}^A, Y_{p,s}^B, Y_{p,s}^C \geq 0 \quad \forall s \in S \tag{4.2x}$$

$$c_{p,s}^u(U_{p,s}) \quad free \quad \forall s \in S \tag{4.2y}$$

For example, suppose player p's investment is desalination and generates a favorable ROI (i.e. $s = 1$). Further, suppose that the water generated alone from desalination $U_{p,1}$ is greater than the threshold i_p^B. Past this threshold, the technology matures bringing down the unit cost to $c_{p,1}^m$ (see Figure 4.3). This desalination example scenario corresponds to specific piecewise activation variables.

In mathematical terms, Expression (4.2w) requires $X_p^{RD} = 1$ for one of $X_{p,1}^A$ or $X_{p,1}^B$ to be non-zero. Furthermore, $Y_{p,1}^A = 0$ because the piecewise segment with slope $c_{p,1}^m$ is assumed to be active per Figure 4.3. This activation is only possible when $X_{p,1}^A = 0$ in (4.2r). Therefore, $X_{p,1}^B = 1$, which allows the weighting terms $Y_{p,1}^B \leq 1$ and $Y_{p,1}^C \leq 1$ per (4.2s) and (4.2t), respectively. Expression (4.2u) requires these weighting terms to sum to one, which constrains $U_{p,1}$ to be between i_p^B and i_p^C in (4.2q).

In summary, Sub-Model 4.4.2 consists of the objective function (4.2b), which includes both the expected payoff (4.2a) and the CVaR risk metric. This objective function is subject to the constraints (4.2c) - (4.2y). Within these constraints, expressions (4.2d) - (4.2o) re-express the constraints from Sub-Model 4.1 in terms of the rolling-horizon approach. The remaining constraints, (4.2c) and (4.2p) - (4.2y) relate to CVaR and the green technology cost curves that were introduced in this section.

Figure 4.4 depicts sample results for Sub-model 4.2 for two different levels of risk tolerance

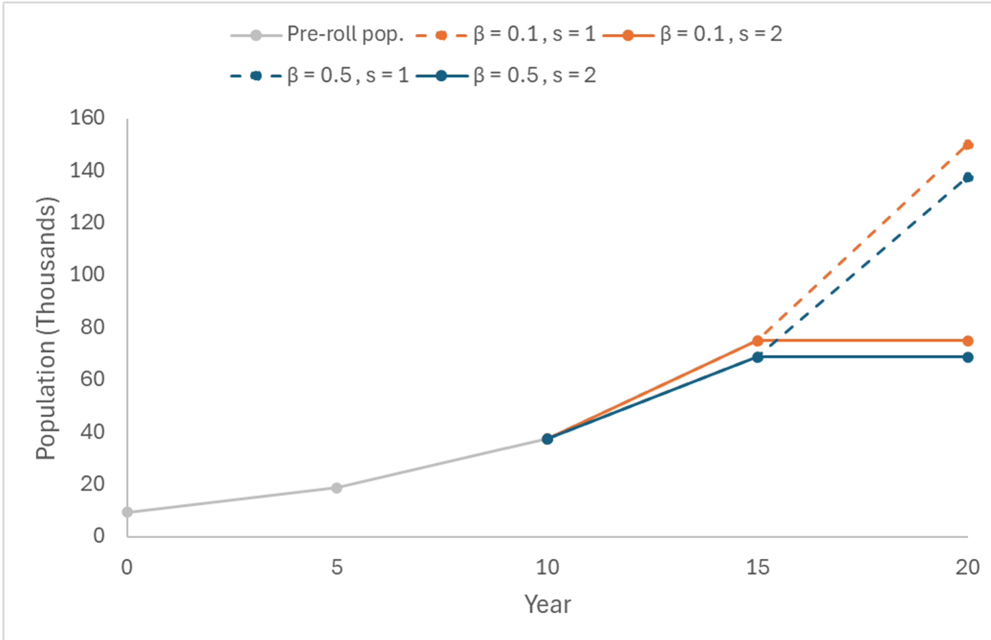


Figure 4.4: Illustrative results for the co-evolution sub-model

(i.e., $\beta_p = 0.1$ and $\beta_p = 0.5$). The input data for these results are provided in Appendix C.2. This chapter assumes that the rolling horizon starts at year 15 (i.e., r=15). Prior to this year, the population levels are low enough to avoid the need for R&D. This chapter also assume that enough capacity (e.g., desalination) can be installed to allow the population to continue growing without a cap.

These results illustrate how Sub-model 4.2 represents the co-evolution of economic/population growth and technology. In $s = 1$, tapping into the unlimited resource is cost-effective enough to maintain the growth of the population and the associated economic benefit. In $s = 2$, the cost of the technology exceeds the benefits of population growth. A solution for this scenario is to maintain the existing population but at a higher cost than for $s = 1$. Both $\beta_p = 0.1$ and $\beta_p = 0.5$ are qualitatively similar in this manner.

Despite these similarities, the population growth rate is smaller for $\beta_p = 0.5$ than $\beta_p =$

0.1 between years 10 - 15. This smaller growth rate results in a lower population to maintain between years 15 - 20. From a risk perspective, maintaining a lower population carries the benefit of reducing the financial burden of procuring resources in the $s = 2$ scenario. However, reducing this financial burden also lowers the economic benefits of population growth in the $s = 1$ scenario.

These results also refine the multi-phase modeling features. Now in each phase (i.e., planning period), technology can be developed, grow in adoption, and reach maturity as in $s = 1$. These phases correspond to the discrete piecewise segments shown in Figure 4.3. Another possible pathway is the stagnation of the technology as in $s = 2$. Thus, the sub-models not only serve to introduce new features but to refine preexisting features introduced in earlier sub-models.

4.4.3 Social Learning Model Features

Sub-model 4.3 considers multiple players, P, who make decisions that are consistent with Sub-model 4.2. Each player $p \in P$ is still a local developer or a local government within a broader region. The region could represent a watershed with a shared surface or groundwater system. Each locality could have a geographical niche for alternative water technologies. For example, a coastal city might be more likely to implement desalination compared to an inland city. Similarly, a farming community on an urban fringe might use recycled wastewater for irrigation.

As will be explained, some adjustments and extensions are made to Sub-model 4.2 to account for the interactions among the players. Only these changes are stated in this section to avoid repeating many unchanged expressions. However, the full formulation for Sub-model 4.3

is provided in Appendix C.3.1. Players share finite resources with each other as one form of interaction. However, social learning is the primary interaction considered per the ST frameworks. This framework accounts for how players learn from the R&D investments of others.

Players can also learn from their own R&D investments over multiple rolls of a rolling-horizon model (e.g., Sub-model 4.2). Mathematically, the Bayesian probabilities $\mathbb{P}_p(s)$ can be updated between each roll using a learning model (e.g., Bayes' Theorem). This approach is called endogenous learning and has been applied to decision-making in energy markets [80]. The details of such an algorithm are excluded from the current study and are left to future research.

To model how the players share finite resources, expressions (4.2f), (4.2g), and (4.2l) are modified, respectively, as follows:

$$\sum_{p' \in P} F^{FS}_{p',r} + H^{FS}_{r} = l + \sum_{p' \in P} W^{FS}_{p',r} \quad (\lambda^{lim1}_{p,r}) \tag{4.3a}$$

$$\sum_{p' \in P} F^{SS}_{p',r+1,s} + H^{SS}_{r+1,s} = l + \sum_{p' \in P} W^{SS}_{p',r+1} \quad (\lambda^{lim2}_{p,r+1,s}) \quad \forall s \in S \tag{4.3b}$$

$$\sum_{p' \in P} W^{SS}_{p',r+1,s} = a^{i} - \sum_{p' \in P} W^{FS}_{p',r} \quad (\lambda^{acc}_{p,r}) \tag{4.3c}$$

where H^{FS}_{r} and $H^{SS}_{r+1,s}$ represent any consumption slack with respect to the natural-resource limit l. The summation index p' indicates that all the players decisions contribute to the depletion of the finite resource. These adjustments make Sub-model 4.3 a type of Generalized Nash Equilibrium model because the players can now affect the constraint set (i.e., resource availability) of others [150].

The players' optimization problems, which incorporate shared resources into Sub-model 4.2, are solved simultaneously. To achieve this, each player's optimization problem is re-expressed as the Karush-Kuhn Tucker (KKT) conditions [21]. The KKT conditions are necessary and sufficient for linear programs (LPs), but Sub-model 4.2 is an example of a MIP. To overcome this limitation, Sub-model 4.3 treats the binary X variables as exogenous decisions to eventually be determined by an upper-level player. Within this context, the shadow prices (i.e., γ and λ terms) are consistent with strong duality as described in [45].

Each combination of binary variables is inspected in tabular form to identify Nash Equilibrium points. To simplify this analysis, only a two player game is considered using Sub-model 4.3. Two player games that can be analyzed in this tabular manner are called bimatrix games. The payoff for each player is the optimal objective function value associated with a particular binary-variable combination. This analysis reveals the benefits of social learning when one or both players invest in R&D at different levels.

In addition to the KKT conditions, other system constraints are included outside of each player's optimization problem. These constraints provide additional details into how the players interact. In this sub-model, the system constraints specify how the finite resources are distributed among the players as well as specify the dynamics of social learning. In related work, system constraints are often related to market-clearing conditions [21] [24].

The first set of system constraints characterize how the players access the shared resources as described in (4.3a) - (4.3c). While the players share these same constraints, their shadow prices (i.e., λ terms) for these constraints could be different. To see this, (4.3a) - (4.3c) are summed over the index p', while the shadow prices are indexed by p. In this chapter's water example, different shadow prices can result from differing costs to pump groundwater.

To model this mathematically, each shadow price is assumed to be a weighted sum of the other player's shadow prices:

$$\lambda_{p,r}^{lim1} = \sum_{p' \neq p} \upsilon_{p,p'}^{FS} \lambda_{p',r}^{lim1} \quad , \quad p < |P| \tag{4.3d}$$

$$\lambda_{p,r+1,s}^{lim2} = \sum_{p' \neq p} \upsilon_{p,p',s}^{SS} \lambda_{p'r+1,s}^{lim2} \quad , \quad p < |P| \quad , \quad s \in S \tag{4.3e}$$

$$\lambda_{p,r}^{acc} = \sum_{p' \neq p} \upsilon_{p,p'}^{A} \lambda_{p',r}^{acc} \quad , \quad p < |P| \tag{4.3f}$$

where the υ terms are non-negative parameters representing these weights. Each set only requires $|P| - 1$ equations to form a square system of equations.

This chapter assumes that the shadow prices must equal zero if there is any slack in the consumption of the finite resource (i.e., $H^{FS} > 0$ or $H^{SS} > 0$). This assumption is reasonable because one or more players leave resources unclaimed in such a case. The following mathematical expressions are thus introduced:

$$0 \leq \sum_{p \in P} \lambda_{p,r}^{lim1} \perp H_r^{FS} \geq 0 \tag{4.3g}$$

$$0 \leq \sum_{p \in P} \lambda_{p,r+1,s}^{lim2} \perp H_{r+1,s}^{SS} \quad \forall s \in S \tag{4.3h}$$

In the first expression, the $\perp$ operator is shorthand for $H_r^{FS}(\sum_{p \in P} \lambda_{p,r}^{lim1}) = 0$ and is called a complementarity relationship. The same meaning applies to this operator in the second expression.

In a qualitative sense, social learning reflects how the one player can learn and/or benefit from the technological investments of other players. For example, a desalination design approach from one location could be repurposed for use in another location saving design costs. Players could also pay to connect to an existing desalination network instead of building a separate facility. Another conception of social learning could be correcting the failures of another player's previous R&D efforts.

These social learning possibilities are relevant because the players may have heterogeneous costs for sustainable technologies. For instance, solar power technologies are likely to be initially most cost-effective in niches that are very sunny and dry. Similarly, wastewater recycling is likely to first emerge near sites with high treatment standards. However innovation in these niches can transfer into the prevailing regimes in most other settings, such as power generation derived from fossil fuels and surface-water depletion.

Social learning is modeled as modification to the piecewise learning curves as shown in Figure 4.5. The function values at the break-points are $c_p^{A'}$ and $c_{p,1}^{B'}$. This reflects no technological investment from the other players. In contrast, Δc_p^A and $\Delta c_{p,1}^B$ represent the maximum decrease of the break-point function values if other players (i.e., $p' \in \{\mathcal{P} : p^{'} \neq p\}$) invest. The impact of one player's investment on that of another is given as $w_{p',p}$. As in Sub-model 4.2, the technology is considered mature at a constant cost $c_{p,1}^m$ beyond break-point B.

A band of possible costs are shown in the grey region of Figure 4.5. The top of this band represents the case when no other players invest. The bottom of the curve represents the case when all other players invest as much as possible. The intermediate region represents all other cases where some players invest at different levels. For example, the red curve for $s = 1$ represents the case where some of the other players invest the fixed cost c_p^A as well as the interval $[0, i_p^B]$.

These social learning relationships are summarized mathematically as the following system

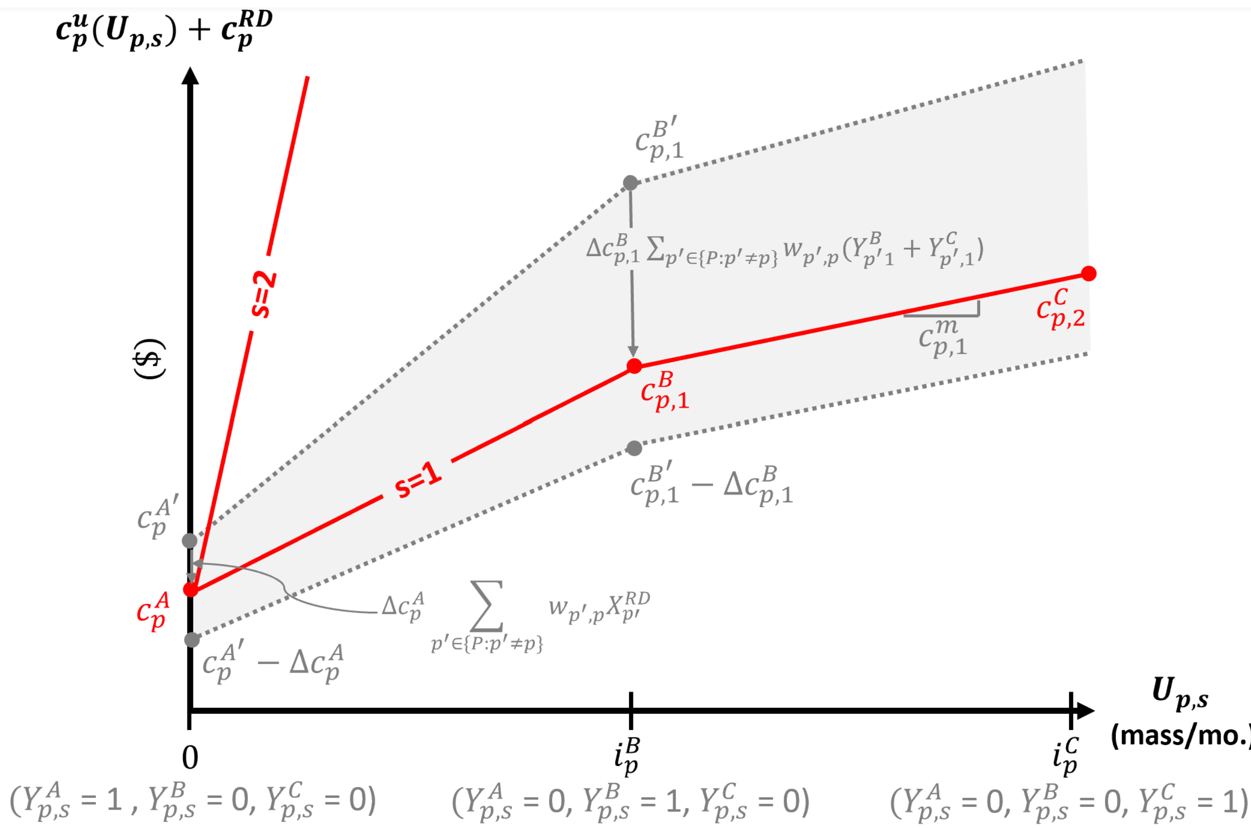


Figure 4.5: Cost curves with social learning aspects

constraints:

$$c_p^{RD} = c_p^A = c_p^{A'} - \Delta c_p^A \sum_{p' \in \{\mathcal{P}:p' \neq p\}} w_{p,p'} X_{p'}^{RD} \tag{4.3i}$$

$$c_{p,s}^B = c_{p,s}^{B'} - \Delta c_{p,s}^B \sum_{p' \in \{\mathcal{P}:p' \neq p\}} w_{p,p'} (Y_{p',s}^B + Y_{p',s}^C) \quad \forall s \in S \tag{4.3j}$$

$$c_{p,s}^C = c_{p,s}^B + c_{p,s}^m (i_p^C - i_p^B) \quad \forall s \in S \tag{4.3k}$$

These system constraints specify how c_p^A, $c_{p,s}^B$, and $c_{p,s}^C$ show up as exogenous data for each player. The piecewise curves start at c_p^A, which also represents the first-stage cost c_p^{RD}. In (4.3i), the *fixed* R&D decisions of other players, $X_{p'}^{RD}$, decrease the *fixed* costs, c_p^A, for player p. Similarly, other players' *continuous* investment decisions (i.e., $U_{p',s}$) decrease the *continuous* investment costs of player p. The sum $Y_{p',s}^B + Y_{p',s}^C$ is a normalized indicator of this continuous investment level in

(4.3j). This sum increases from zero to one as $U_{p',s}$ approaches $i_{p'}^B$.

In summary, Sub-model 4.3 consists of KKT conditions from multiple players' optimization problems and system constraints. These constraints govern the interactions among the players. The KKT conditions for each player are derived from Sub-model 4.2 except that 1) the binary decisions are taken as data and 2) Expressions (4.2f), (4.2g), and (4.2l) are replaced with (4.3a), (4.3b), and (4.3c), respectively. The system constraints consist of (4.3i) - (4.3h). Sub-model 4.3 is solved as a mixed-complementary problem (MCP) [21]. The full mathematical details are provided in Appendix C.3.1.

Sample results for Sub-model 4.3 are presented for a game involving two players (e.g., two cities). These results are summarized as a bimatrix game in Tables 4.1 and 4.2 for players 1 and 2, respectively. The binary variables for technology investment are the strategies. The payoffs of these strategies are calculated from the equilibrium solutions of Sub-model 4.3 by enumeration. The input data for these sample results is provided in Appendix C.3.2.

The players are identical in terms of the input data with two exceptions. First, player 2 has lower technology investment costs than player 1. In the desalination example, this could mean that player 2 is closer to the ocean. Second, player 1 is assumed to have a slightly smaller shadow price for the finite resource in the first stage (i.e., $v_{1,2}^{FS} = 0.5$). In the water context, this could mean that player 1's distance from the ocean could place it upstream on a river relative to player 2.

The bold-text numbers in these tables represent the equilibrium solutions of this bimatrix game. Although four are shown, they represent four ways to arrive at the same technology investment outcome. This redundancy exists because the equilibrium solution for $U_{1,2} = i_1^B$ and $U_{2,2} = i_2^B$. Either X^A or X^B can be used to activate i_p^B because it is located at the cusp of the two

Table 4.1: Payoffs for player 1 computed from Sub-Model 4.3 (Thousands of Dollars). Player 1 seeks to maximize their payoff. For a given s, the term $X^A_{1,s} = 1$ means that $U_{1,s} \leq i^B_1$. In contrast, $X^B_{1,s} = 1$ means that $U_{1,s} \geq i^B_1$.

	$X_2^{RD} = 0$	$X^A_{2,1} = 1$ $X^B_{2,1} = 0$ $X^A_{2,2} = 1$ $X^B_{2,2} = 0$	$X^A_{2,1} = 1$ $X^B_{2,1} = 0$ $X^A_{2,2} = 0$ $X^B_{2,2} = 1$	$X^A_{2,1} = 0$ $X^B_{2,1} = 1$ $X^A_{2,2} = 1$ $X^B_{2,2} = 0$	$X^A_{2,1} = 0$ $X^B_{2,1} = 1$ $X^A_{2,2} = 0$ $X^B_{2,2} = 1$
$X_1^{RD} = 0$	\$641.25	\$641.25	\$641.25	\$709.59	\$641.25
$X^A_{1,1} = 1$ $X^B_{1,1} = 0$ $X^A_{1,2} = 1$ $X^B_{1,2} = 0$	\$25.06	\$435.00	\$435.00	\$469.31	\$469.31
$X^A_{1,1} = 1$ $X^B_{1,1} = 0$ $X^A_{1,2} = 0$ $X^B_{1,2} = 1$	-\$172.66	\$215.63	\$332.63	\$469.31	\$469.31
$X^A_{1,1} = 0$ $X^B_{1,1} = 1$ $X^A_{1,2} = 1$ $X^B_{1,2} = 0$	\$343.44	\$979.31	\$1,050.00	**\$1,056.28**	**\$1,056.28**
$X^A_{1,1} = 0$ $X^B_{1,1} = 1$ $X^A_{1,2} = 0$ $X^B_{1,2} = 1$	\$343.44	\$979.31	\$1,018.31	**\$1,056.28**	**\$1,056.28**

Table 4.2: Payoffs for player 2 computed from Sub-Model 4.3 (Thousands of Dollars). Player 2 seeks to maximize their payoff. For a given s, the term $X^A_{2,s} = 1$ means that $U_{2,s} \leq i^B_2$. In contrast, $X^B_{2,s} = 1$ means that $U_{2,s} \geq i^B_2$.

	$X_2^{RD} = 0$	$X^A_{2,1} = 1$ $X^B_{2,1} = 0$ $X^A_{2,2} = 1$ $X^B_{2,2} = 0$	$X^A_{2,1} = 1$ $X^B_{2,1} = 0$ $X^A_{2,2} = 0$ $X^B_{2,2} = 1$	$X^A_{2,1} = 0$ $X^B_{2,1} = 1$ $X^A_{2,2} = 1$ $X^B_{2,2} = 0$	$X^A_{2,1} = 0$ $X^B_{2,1} = 1$ $X^A_{2,2} = 0$ $X^B_{2,2} = 1$
$X_1^{RD} = 0$	\$641.25	\$692.00	\$667.63	\$1,005.31	\$1,118.94
$X^A_{1,1} = 1$ $X^B_{1,1} = 0$ $X^A_{1,2} = 1$ $X^B_{1,2} = 0$	\$846.28	\$806.33	\$806.33	\$1,279.81	\$1,279.81
$X^A_{1,1} = 1$ $X^B_{1,1} = 0$ $X^A_{1,2} = 0$ $X^B_{1,2} = 1$	\$945.00	\$906.88	\$877.63	\$1,279.81	\$1,279.81
$X^A_{1,1} = 0$ $X^B_{1,1} = 1$ $X^A_{1,2} = 1$ $X^B_{1,2} = 0$	\$709.59	\$611.56	\$579.88	**\$730.81**	**\$730.81**
$X^A_{1,1} = 0$ $X^B_{1,1} = 1$ $X^A_{1,2} = 0$ $X^B_{1,2} = 1$	\$709.59	\$611.56	\$601.81	**\$730.81**	**\$730.81**

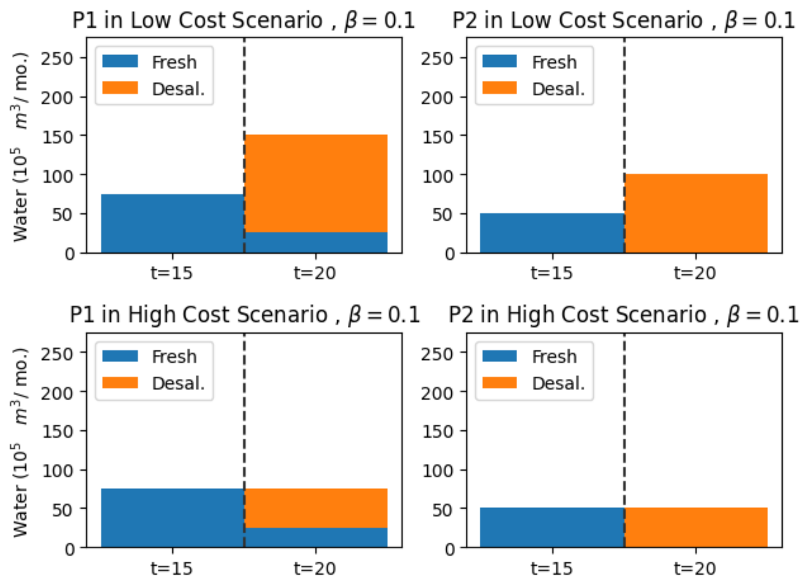
piecewise intervals $[0, i_p^B]$ and $[i_p^B, i_p^C]$. For this chapter's desalination example, $i_p^B = 50$ units (e.g., $10^5 \quad m^3/mo.$ of water).

Observing the payoffs in Table 4.1 indicates how the two players interact. Player 1's maximum payoffs occur at the equilibrium solutions (i.e., $1,192.97K). These payoffs coincide with player 2 investing in desalination. When player 2 does not invest in R&D at all (i.e., $X_2^{RD} = 0$), the best strategy player 1 can take is to also not invest in R&D and receive a lower payoff of $641.25 K.

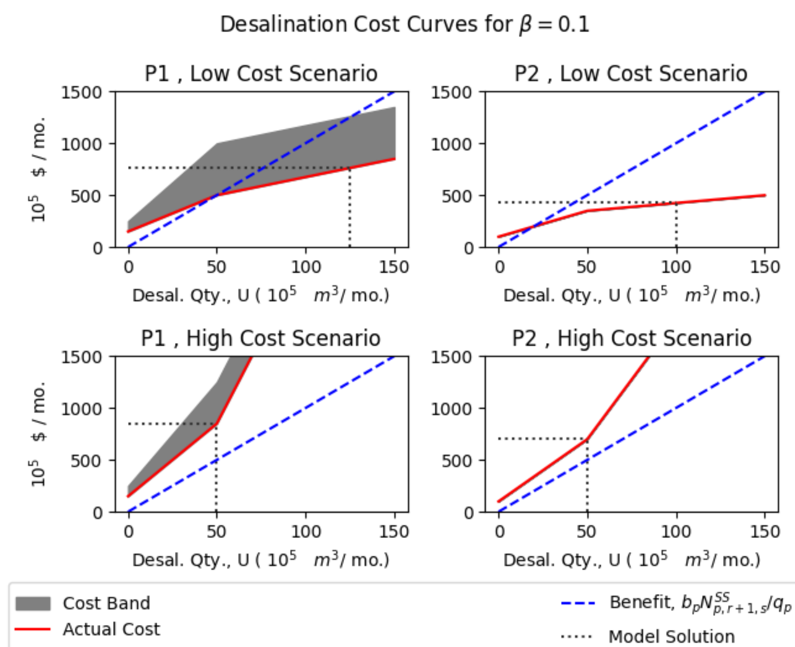
Figure 4.6 graphically depicts these results within the context of this chapter's desalination example. Sub-figure 4.6a depicts the quantities of fresh and desalinated water for each player, scenario, and time period in the rolling horizon. Sub-figure 4.6b depicts the technology cost curves for desalination, which are consistent with Figure 4.5. Each sub-figure has four frames where each frame represents a scenario for a particular player. In Sub-Figure 4.6a, each frame is further subdivided into the two time periods of the rolling horizon. In Sub-Figure 4.6b, the time period is implicitly $r = t + 1$.

Figure 4.6a illustrates the interplay between access to the finite resource and the utilization of the practically unlimited resource. Player 1 uses more freshwater (i.e., F) in the first stage (i.e., $t = r = 15$) than player 2 because player 1 has a lower finite resource shadow price (i.e., $\lambda_{1,r}^{lim1} = 0.9\lambda_{2,r}^{lim1}$). This resource advantage allows player 1's population to grow larger than player 2's between years $t = 15$ and $t = 20$. Consequentially, player 1 can also use more desalination (i.e., U) than player 2 for population growth in $t = 20$ onwards.

Figure 4.6b shows the specifics of social learning between the two players at the equilibrium solutions. In the low-cost scenario (i.e., $s = 1$), player 2, installs $100 \quad 10^5 m^3/mo.$ of desalination capacity. This decision is rational because the red technology cost curve is always



(a) Resource usage corresponding to the bimatrix game equilibrium solutions



(b) Social learning related to the technology cost curves in the bimatrix game equilibrium solutions

Figure 4.6: Desalination quantity and cost relationships for the Sub-model 4.3 example

lower than the dashed-blue benefit curve. This curve is simply the population benefit re-expressed in terms of resource consumption: $b_p N^{SS}_{p,r+1,s}/q_p$. In terms of social learning, player 2's decision also brings the technology cost below the benefit for player 1.

The gray cost bands in Figure 4.6b indicate a uni-directional social learning relationship. Player 2 does not have a cost band because they are assumed to implement desalination independent of player 1's investments. In terms of the ST literature, player 2 represents the desalination niche (e.g., coastal area). In contrast, player 1's cost band is dependent on the investment actions of player 2.

For instance, suppose that player 2's desalination investments lower the cost of membrane filtration technology to treat sea water. Player 1 is located farther inland and can't directly apply the technology in the same way. However, suppose player 1 can adapt the cheaper membrane filtration technology for another purpose. For example, cheaper membrane-treatment-technologies could be used to treat brackish water (i.e., less salty) water to drinking-water standards.

Figure 4.6b also shows the high cost, technology-stagnation scenario (i.e., $s = 2$) in the lower-two frames. For both players, the cost to implement desalination is greater than the benefit of population growth. Player 2's cost is marginally higher than player 1's cost in this scenario. However, both players implement enough desalination to maintain the $t = 15$ population levels at $t = 20$. This implementation avoids incurring a high cost associated with emigration out of the region.

4.4.4 Multi-Level Model Features

The inequity of resource use in Figure 4.6a motivates the analysis of resource-allocation policies. To achieve this, multi-level features are added to Sub-model 4.3 to form the full bi-level optimization model. This chapter's bi-level optimization problem adds a single, upper-level, regional policymaker to allocate resources among the lower-level, players. This upper-level player could be a state or national government who is responsible for: 1) the equitable distribution of resources within their jurisdiction, and 2) defining R&D goals for alternative resources (e.g., renewable energy, desalination).

In terms of resource distribution, the policymaker allocates $L^{FS}_{p,r}$ to player p in the first stage. Similarly, they allocate $L^{SS}_{p,r+1,s}$ finite resources (e.g., water withdrawal permits) to player p in the second stage on the basis of technology outcome scenario s. These allocations replace the shared-resource constraints (4.3a) and (4.3b) with the following expressions:

$$F^{FS}_{p,r} \leq L^{FS}_{p,r} \quad (\gamma^{lim1}_{p,r}) \tag{4.4}$$

$$F^{ss}_{p,r+1,s} \leq L^{SS}_{p,r+1,s} \quad (\gamma^{lim1}_{p,r+1,s}) \quad \forall s \in S \tag{4.5}$$

Consequently, the removal of the shared-resource constraints eliminates the Generalized Nash aspects of Sub-model 4.3.

This direct allocation approach allows several expressions to be omitted. Expression (4.3c) is eliminated completely because withdrawals from the accumulated resource are part of each local developer's allocation. Similarly, the system constraints (4.3d) - (4.3h) are omitted because the policy maker's allocation decisions indirectly influence the shadow prices for the finite resource.

The policymaker also decides the binary variables related to technology that were treated as bimatrix strategies in Sub-model 4.3. These decisions can be interpreted as a requirement for the lower-level players as a condition on their finite-resource allocation. For instance, having $X_p^{RD} = 1$ obligates player p to pay the fixed R&D costs for the technology. Furthermore, for a given scenario s, having $X_{p,s}^B = 1$ indicates a minimum adoption level i_p^B for $U_{p,s}$.

This interpretation can be justified mathematically. Per (4.2u), $X_p^{RD} = 1$ requires the sum of the Y terms to equal one. Assuming the piecewise structure in Figure 4.5, the minimum cost of this requirement is the fixed value c_p^A, which corresponds to $Y_{p,s}^A = 1$. However, this minimum cost increases when $X_{p,s}^B = 1$. In this situation, (4.2w) requires $X_{p,s}^A = 0$. Thus, $Y_{p,s}^A = 0$ per (4.2r). Using a parallel argument to the $X_{p,s}^B = 0$ case, the minimum cost is now $c_{p,s}^B$ with $U_{p,s} > 0$.

The following KKT stationary conditions (4.6) and KKT feasibility conditions (4.7) mathematically characterize how the local developers respond to the policymaker's decisions. These KKT conditions are identical to those used in Sub-model 4.3 save the adjustments noted in (4.4) and (4.5). Thus, these KKT conditions are still necessary and sufficient conditions for optimal solutions for the lower level players.

$$0 \leq q_p \gamma_{p,r}^{dem1} + \gamma_{p,r}^{max1} + \sum_{s \in S} (\gamma_{p,r+1,s}^{min2} - g_p \gamma_{p,r+1,s}^{max2}) \\ - b_p((1-\beta_p) + \sum_{s \in S} \gamma_{p,s}^{rsk}) - \gamma_{p,r}^{min1} \perp N_{p,r}^{FS} \geq 0 \quad (4.6a)$$

$$0 \leq q_p \gamma^{dem2}_{p,r+1,s} + \gamma^{max2}_{p,r+1,s} - \gamma^{min2}_{p,r+1,s} - d_{p,r+1} b_p (\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) \perp N^{SS}_{p,r+1,s} \geq 0 \quad \forall s \in S \tag{4.6b}$$

$$0 \leq c^e_p((1-\beta_p) + \sum_{s \in S} \gamma^{rsk}_{p,s}) - \gamma^{min1}_{p,r} \perp E^{FS}_{p,r} \geq 0 \tag{4.6c}$$

$$0 \leq d_{p,r+1} c^e_p (\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \gamma^{min2}_{p,r+1,s} \perp E^{SS}_{p,r+1,s} \geq 0 \quad \forall s \in S \tag{4.6d}$$

$$0 \leq c^f_p((1-\beta_p) + \sum_{s \in S} \gamma^{rsk}_{p,s}) + \gamma^{lim1}_{p,r} - \gamma^{dem1}_{p,r} \perp F^{FS}_{p,r} \geq 0 \tag{4.6e}$$

$$0 \leq d_{p,r+1} c^f_p (\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) + \gamma^{lim2}_{p,r+1,s} - \gamma^{dem2}_{p,r+1,s} \perp F^{SS}_{p,r+1,s} \geq 0 \quad \forall s \in S \tag{4.6f}$$

$$0 \leq \lambda^u_{p,s} - \gamma^{dem2}_{p,r+1,s} \perp U_{p,s} \geq 0 \quad \forall s \in S \tag{4.6g}$$

$$0 \leq \frac{\beta_p \mathbb{P}_p(s)}{1-\alpha_p} - \gamma^{rsk}_{p,s} \perp V_{p,s} \geq 0 \quad \forall s \in S \tag{4.6h}$$

$$\sum_{s \in S} \gamma^{rsk}_{p,s} - \beta_p = 0 \quad , \quad Z_p \quad free \tag{4.6i}$$

$$0 \leq \gamma^A_{p,s} + \lambda^{rd}_{p,s} + c^A_p \lambda^{pw}_{p,s} - i^A_p \lambda^u_{p,s} \perp Y^A_{p,s} \geq 0 \quad \forall s \in S \tag{4.6j}$$

$$0 \leq \gamma^B_{p,s} + \lambda^{rd}_{p,s} + c^B_{p,s} \lambda^{pw}_{p,s} - i^B_p \lambda^u_{p,s} \perp Y^B_{p,s} \geq 0 \quad \forall s \in S \tag{4.6k}$$

$$0 \leq \gamma^C_{p,s} + \lambda^{rd}_{p,s} + c^C_{p,s} \lambda^{pw}_{p,s} - i^C_p \lambda^u_{p,s} \perp Y^C_{p,s} \geq 0 \quad \forall s \in S \tag{4.6l}$$

$$d_{p,r+1}(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \lambda^{pw}_{p,s} = 0 \quad , \quad c^u_{p,s} \quad free \quad \forall s \in S \tag{4.6m}$$

$$0 \leq V_{p,s} - Z_p + \Big(b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p +$$
$$d_{p,r+1}\Big(b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s})\Big)\Big) \perp \gamma^{rsk}_{p,s} \geq 0 \quad \forall s \in S \quad (4.7a)$$

$$0 \leq F^{FS}_{p,r} - q_p N^{FS}_{p,r} \perp \gamma^{dem1}_{p,r} \geq 0 \quad (4.7b)$$

$$0 \leq F^{SS}_{p,r+1,s} + U_{p,s} - q_p N^{SS}_{p,r+1,s} \perp \gamma^{dem2}_{p,r+1,s} \geq 0 \quad \forall s \in S \quad (4.7c)$$

$$0 \leq L^{FS}_{p,r} - F^{FS}_{p,r} \perp \gamma^{lim1}_{p,r} \geq 0 \quad (4.7d)$$

$$0 \leq L^{SS}_{p,r+1,s} - F^{SS}_{p,r+1,s} \perp \gamma^{lim2}_{p,r+1,s} \geq 0 \quad \forall s \in S \quad (4.7e)$$

$$0 \leq g_p n^i_p - N^{FS}_{p,r} \perp \gamma^{max1}_{p,r} \geq 0 \quad (4.7f)$$

$$0 \leq g_p N^{FS}_{p,r} - N^{SS}_{p,r+1,s} \perp \gamma^{max2}_{p,r+1,s} \geq 0 \quad \forall s \in S \quad (4.7g)$$

$$0 \leq N^{FS}_{p,r} + E^{FS}_{p,r} - n^i_p \perp \gamma^{min1}_{p,r} \geq 0 \quad (4.7h)$$

$$0 \leq N^{SS}_{p,r+1,s} + E^{SS}_{p,r+1,s} - N^{FS}_{p,r} \perp \gamma^{min2}_{p,r+1,s} \geq 0 \quad \forall s \in S \quad (4.7i)$$

$$c^u_{p,s}(U_{p,s}) = c^A_p Y^A_{p,s} + c^B_{p,s} Y^B_{p,s} + c^C_{p,s} Y^C_{p,s} - c^{RD}_p X^{RD}_p \quad , \quad \lambda^{pw}_{p,s} \quad free \quad \forall s \in S \quad (4.7j)$$

$$U_{p,s} = i^A_p Y^A_{p,s} + i^B_p Y^B_{p,s} + i^C_p Y^C_{p,s} \quad , \quad \lambda^u_{p,s} \quad free \quad \forall s \in S \quad (4.7k)$$

$$0 \leq X^A_{p,s} - Y^A_{p,s} \perp \gamma^A_{p,s} \geq 0 \quad \forall s \in S \quad (4.7l)$$

$$0 \leq X^A_{p,s} + X^B_{p,s} - Y^B_{p,s} \perp \gamma^B_{p,s} \geq 0 \quad \forall s \in S \quad (4.7m)$$

$$0 \leq X^B_{p,s} - Y^C_{p,s} \perp \gamma^C_{p,s} \geq 0 \quad \forall s \in S \tag{4.7n}$$

$$Y^A_{p,s} + Y^B_{p,s} + Y^C_{p,s} = X^{RD}_p \quad , \quad \lambda^{rd}_{p,s} \quad free \quad \forall s \in S \tag{4.7o}$$

Program (4.8) formalizes how the upper-level policymaker makes their allocation decisions. The variables without subscripts are vectors that contain all the related variables as components for notational simplicity. In (4.8a), the policymaker seeks to maximize a social welfare metric, which is the sum across the lower-level objective functions. Such an objective function is known as aggregate optimization [14] [25]. The KKT conditions (4.6) and (4.7) are subsumed as equilibrium constraints. Expressions (4.8c) - (4.8m) represent additional constraints on the policymaker.

$$\max_{L^{FS},W^{FS},L^{SS},W^{SS},A,X^{RD},X^A,X^B} \sum_{p \in P} \Big(1-\beta_p\Big) \Big(b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p + d_{p,r+1} \sum_{s \in S} \mathbb{P}_p(s) \Big($$
$$b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s})\Big)\Big) + \beta_p \left(Z_p - \frac{1}{1-\alpha_p} \sum_{s \in S} \mathbb{P}_p(s) V_{p,s} \right) \tag{4.8a}$$

s.t.

$$\{N^{FS}, N^{SS}, E^{FS}, E^{SS}, F^{FS}, F^{SS}, U, Y^A, Y^B, Y^C\} \in KKT(L^{FS}, L^{SS}, X^{RD}, X^A, X^B) \tag{4.8b}$$

$$\sum_{p \in P} L^{FS}_{p,r} = l + W^{FS}_r \tag{4.8c}$$

$$\sum_{p \in P} L^{SS}_{p,r+1,s} = l + W^{SS}_{r+1} \quad \forall s \in S \tag{4.8d}$$

$$A_{r+1} = a^i - W_r^{FS} \tag{4.8e}$$

$$W_{r+1}^{SS} \leq A_{r+1} \tag{4.8f}$$

$$X_p^{RD} \in \{0, 1\} \tag{4.8g}$$

$$X_{p,s}^A, X_{p,s}^B \in \{0, 1\} \quad \forall s \in S \tag{4.8h}$$

$$X_{p,s}^A + X_{p,s}^B = X_p^{RD} \quad \forall (p, s) \in S \times P \tag{4.8i}$$

$$c_p^{RD} = c_p^A = c_p^{A'} - \Delta c_p^A \sum_{p' \in \{\mathcal{P}: p' \neq p\}} w_{p,p'} X_{p'}^{RD} \tag{4.8j}$$

$$c_{p,s}^B = c_{p,s}^{B'} - \Delta c_{p,s}^B \sum_{p' \in \{\mathcal{P}: p' \neq p\}} w_{p,p'} (Y_{p',s}^B + Y_{p',s}^C) \tag{4.8k}$$

$$c_{p,s}^C = c_{p,s}^B + c_{p,s}^m (i_p^C - i_p^B) \tag{4.8l}$$

$$L^{FS}, L^{SS}, W, A \geq 0 \tag{4.8m}$$

Constraints (4.8c) - (4.8f) are analogous to the shared-resource constraints from Sub-Model 4.3. Constraints (4.8c) and (4.8d) state that the sum of the allocations must equal the limit l plus any withdrawals from the accumulated reserve. These constraints apply to the first and second stages, respectively. Constraints (4.8e) and (4.8f) are the same as (4.2l) and (4.2m) in Sub-model 4.2 except that the policymaker controls them.

Lastly, Constraints (4.8g) - (4.8l) are the remaining system constraints carried over from Sub-model 4.3. They represent the social learning aspects of technology investment. As previously mentioned, the Sub-model 4.3 system constraints that relate to shadow prices are omitted from this upper-level problem.

4.5 Water Resources Illustrative Results

4.5.1 Overview

Water-Resource transitions parallel energy systems, the latter having received a lot of attention in the literature [151]. For instance, both systems have a limited quantity of economically accessible resources (e.g., fossil fuels, freshwater). Furthermore, these systems have additional resources that are very abundant but are difficult to access. In energy systems, these are renewable energy sources such as wind and solar. In water systems, the equivalent involves water treatment of alternative water sources such as saltwater or wastewater.

This illustrative example focuses on desalinated seawater because the scale of its future implementation is a major unknown in water policy. Desalination is an example of a large, capital improvement that often generates a large quantity of water supply. In this sense, desalination is similar to other physical infrastructure developed widely in the twentieth century such as dams, reservoirs, and large water treatment facilities. Physical capital alone cannot solve all water-resource-related problems because unlimited water extraction is not likely to be sustainable in the long term [152].

Because of this sustainability concern, some researchers emphasize behavioral changes (i.e., social capital) over physical capital. For example, home retrofits can increase the efficiency of water fixtures or enable wastewater to be recycled for gardening. Similarly, market-based approaches like dynamic water pricing can be used to regulate water demand. Solutions that emphasize these behavioral changes over hard infrastructure investment are called "soft path" solutions [152].

Both hard and soft infrastructure need to be considered together in water policies. For example, the premature adoption of water desalination can hinder the adoption of alternatives like wastewater reuse [153] [154]. On the other hand, a degree of abundance is necessary to create the conditions for intermediate scarcity, which is necessary for soft solutions to actually work [15]. Desalination can provide this water abundance in some settings where it would otherwise be lacking.

Desalination occupies a water-supply niche in high-income, water-scarce countries, but obstacles still exist for larger-scale deployment [117]. First, removing salt from water is very energy-intensive. Second, the desalination process yields hyper-concentrated brine, which requires environmentally responsible disposal. The management of desalination brine is part of a broader set of challenges with wastewater resource recovery in general [155]. Thus, in most cases, the prevailing regime for water supply is catered to freshwater treatment and distribution.

Within this context, these illustrative results use the model of Section 4.4 to explore the role of desalination in sustainability transitions. Table 4.3 provides an interpretation of the abstract model terminology as applied to these results. The subscripts for these terms are dropped for parsimony. In general, the model terms that are related to the finite resource pertain to traditional freshwater sources. In contrast, the terms that are related to the alternative, unlimited resource pertain to desalination.

Furthermore, Table 4.3 assumes that the environmental externalities of brine management are priced into the desalination costs. This assumption is aspirational for sustainability transitions and does not necessarily reflect current practice. Regulating salinity where brine mixes with seawater is a common approach for addressing these externalities. However, brine-disposal regulations vary considerably around the world [156]. Finding cost-effective solutions for these

Table 4.3: Interpretation of this chapter's ST model for water-resource systems

Term(s)	Type	General Description	Water-Resources Interpretation
$t = r, t = r + 1$	Set Element(s)	Time periods within the rolling horizon.	Interval between developments of water supply master plans (e.g., 5-10 years)
$s = 1$	Set Element(s)	Transition scenario where the technology improves	R&D yields promising technology to decrease brine management cost
$s = 2$	Set Element(s)	Scenario where technology stagnates (i.e., no transition)	R&D does not yield promising brine management technology
l	Parameter	Quantity of the finite resource	Replinishable supply of fresh water sources (e.g., rivers, lakes, groundwater)
a^i	Parameter	Initial accumulation of the finite resource at the start of the rolling horizon	Non-replenishable supply of fresh water sources (e.g., deep groundwater reserves)
q	Parameter	Resource required per unit of population supported	Water-use per capita
c^f	Parameter	Cost of accessing the finite resource	Marginal cost to treat and distribute fresh water sources
F^{FS}, F^{SS}	Lower-Level Variable	Finite resources consumed across all players in the first and second stages, respectively	Average monthly fresh water withdrawals in the current and next planning period, respectively
U	Lower-Level Variable	The alternative, unlimited resource that is harnessed using technology	Desalinated seawater
c^A	Variable	Cost at the first piecewise breakpoint	Fixed cost to install desalination facilities and R&D for brine management
c^B	Variable	Cost at the second piecewise breakpoint	Minimum investment required to discover cheaper brine management alternatives
c^C	Variable	Cost at the third piecewise breakpoint	Maximum desalination investment possible given limitations to brine discharge
w	Parameter	Weight relating the impact of one player's technology investment to another	Making minor adjustments to existing desalination designs, inland communities connecting pipelines to a desalination network
c^m	Parameter	Marginal cost of the technology after reaching maturity	Marginal cost of mature desalination technology

regulations is also challenging. Empirical optimization of brine treatment and CO_2 sequestration interactions has been modeled using non-convex functions involving sodium hydroxide dosing, salinity, and CO_2 flow rate [157].

At the start of the rolling horizon, there are two players that are identical except for their desalination cost curves. This is done to investigate how technology influences water allocation policy keeping all other factors equal. For illustrative purposes, assume that the player with the less expensive desalination cost curve manages a coastal region. In contrast, the player with the more expensive cost curve manages an inland region. The illustrative input data is identical to the Sub-model 4.3 data except that the v weighting terms are omitted.

This illustrative model was solved as a specific instance of the bi-level optimization problem (Program 4.8). It was compiled and solved in GAMS using an application programming interface with Python [1]. The solution procedure used a decomposition approach [158] to reformulate the complementary relationships in (4.8b). Lastly, the Solving Constraint Integer Programs (SCIP) algorithm [159] computed the global solutions to Program 4.8. Several iterations were performed for different values of β_p to see how the results were sensitive to varying degrees of risk aversion by the two players.

The reformulation is provided in Appendix C.4.4. The inequalities associated with the complementarity constraints are re-expressed as equalities with non-negative slack variables (denoted as K). Additionally, two additional variables, I and J are introduced as necessary elements of the decomposition. For this reformulation to work, the following condition must hold: I, J, or both I and J must equal zero. Such a condition where only one term can be non-zero is called a special ordered set of type one (i.e., SOS1).

These new variables I, J and K all have superscripts and subscripts to identify the complementarity relationship in question. The shorthand $(I, J) \in SOS1$ indicates that I and J that share the same superscript and subscript must be SOS1. For example, $I^U_{2,1}$, $J^U_{2,1}$, and $K^U_{2,1}$ all apply to the KKT conditions for $U_{2,1}$. Additionally, only one of $I^U_{2,1}$ and $J^U_{2,1}$ can be non-zero.

4.5.2 Results

Figure 4.7 summarizes the payoffs on the horizontal axis versus CVaR (i.e., risk) on the vertical axis. Representative values of $\beta_p \in \{0.1, 0.5, 0.7, 0.8\} \quad \forall p \in \mathcal{P}$ are depicted. The solutions for $\beta_p = 0.5, 0.7$ are the same. Interestingly, varying β_p does not yield Pareto-dominant solutions for both players as is the case for a single decision maker. For player 1, the moderately

[1] www.gams.com/

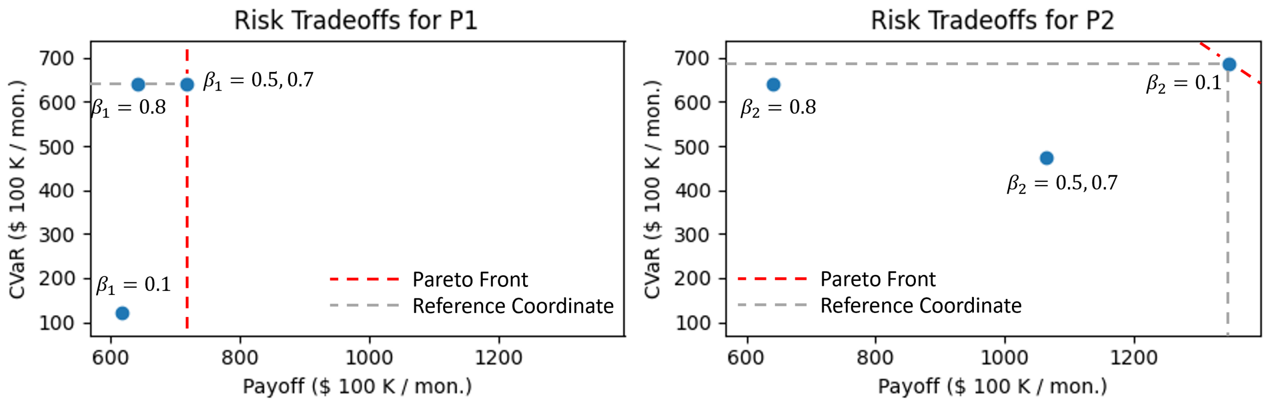


Figure 4.7: Risk trade-offs and overview of model runs

risk-sensitive solution (i.e., $\beta_p \in \{0.5, 0.7\}$) yields a Pareto-dominant solution. For player 2, only the risk-tolerant solution (i.e., $\beta_p = 0.1$) yields a Pareto-dominant solution. [2]

Additionally, comparing the left and right frames of Figure 4.7 shows that risk aversion decreases the differences in payoff and CVaR between the two players. For instance, player 1 and player 2 have identical payoffs and risk when $\beta_p = 0.8$. In contrast, the payoffs are significantly higher for player 2 than player 1 when risk aversion is lower (i.e., $\beta_p \in \{0.1, 0.5, 0.7\}$). The most pronounced difference in payoffs occurs at $\beta_p = 0.1$. These results support the notion that risk aversion leads to greater equity between the players.

Figure 4.8 explains why $\beta_p = 0.1$ is so favorable for player 2. As shown in Figure 4.8a, player 1 and player 2's first-stage water consumption levels are reversed relative to the equilibrium solution (see Figure 4.6a). Specifically, player 1 consumes 50 units of water in the first stage while player 2 consumes 75 units. The upper-level policymaker allocates water in this manner to maximize player 2's population growth and desalination use in $s = 1$.

Maximizing player 2's population growth is optimal across both players because player

[2]Risk-tolerant in this context corresponds to small, non-zero values of β_p that maximize CVaR in the objective function but otherwise preserve risk-neutral solutions. Specifically, the solution for $\beta_p = 0.1$ has the same expected payoffs, desalination quantities, and populations as the true risk-neutral solution (i.e., $\beta_p = 0.0$). However, CVaR receives no weight in this risk-neutral objective function and thus is not necessarily maximized.

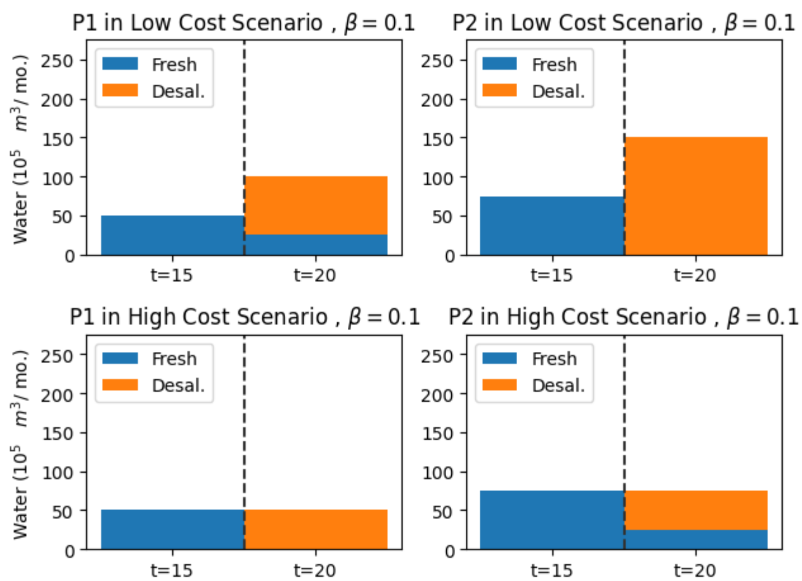
2 has the lower desalination costs (Figure 4.8b). These lower costs translate into a higher net benefit for player 2 because the unit population benefit, b_p, is the same for both players. The desalination costs are incurred because the freshwater reserves are insufficient to maintain the population growth levels of both players.

When $\beta_p > 0.1$, the policymaker tends to decrease player 2's freshwater allocation in $t = 15$ as their risk aversion to scenario $s = 2$ increases (see Figure 4.9). Such an allocation pattern is Pareto-dominant for player 1 when $\beta_p = 0.5, 0.7$. In such a case, player 2 invests less into desalination, which means less social learning benefit to player 1. However, player 2 also receives a lower first-stage allocation compared to Figure 4.6a. This reduced allocation to player 2 frees up additional freshwater for player 1's population growth. Thus, the value of additional freshwater is more valuable to player 1 than the lower desalination cost when $\beta_p = 0.1$.

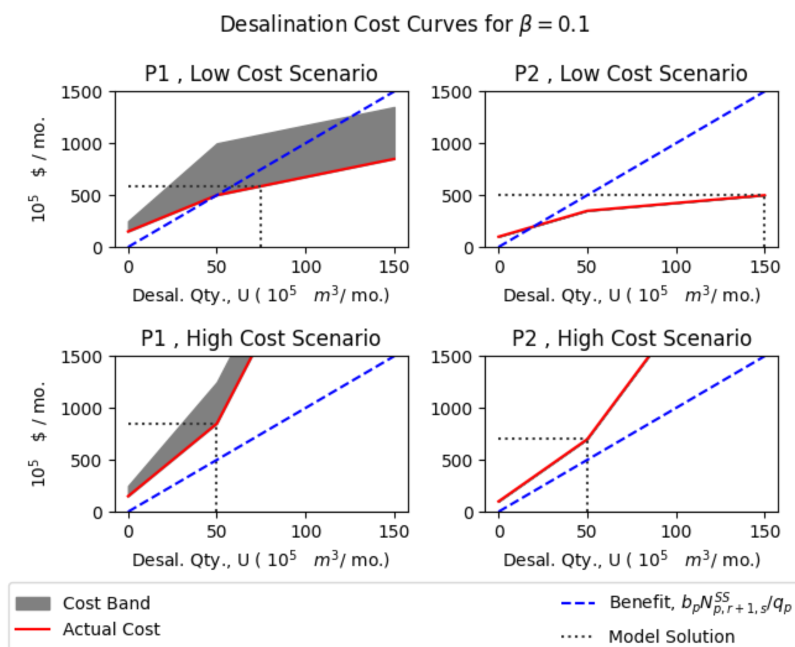
When $\beta_p = 0.8$, both players receive the same allocation and avoid investing in desalination at all (see Figure 4.10). This occurs because the risk of technology stagnation $s = 2$ is intolerable. Thus, the differences between the two players in terms of desalination cost is inconsequential. Given these equal allocations, equity becomes the top consideration over growth at high values of β_p.

4.6 Conclusions

In conclusion, the degree to which economic growth is compatible with sustainability transitions largely depends on one's risk tolerance to technological complexity. A risk-tolerant stance tends to suggest an underlying compatibility with economic growth and sustainability transitions. Additionally, the risk-tolerant stance tends to disregard equity considerations because of cost ad-

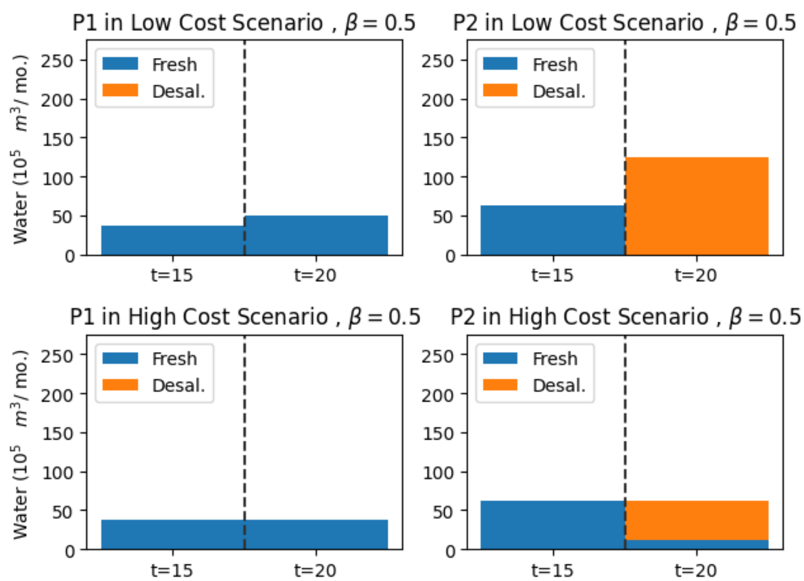


(a) Resource usage in the final model

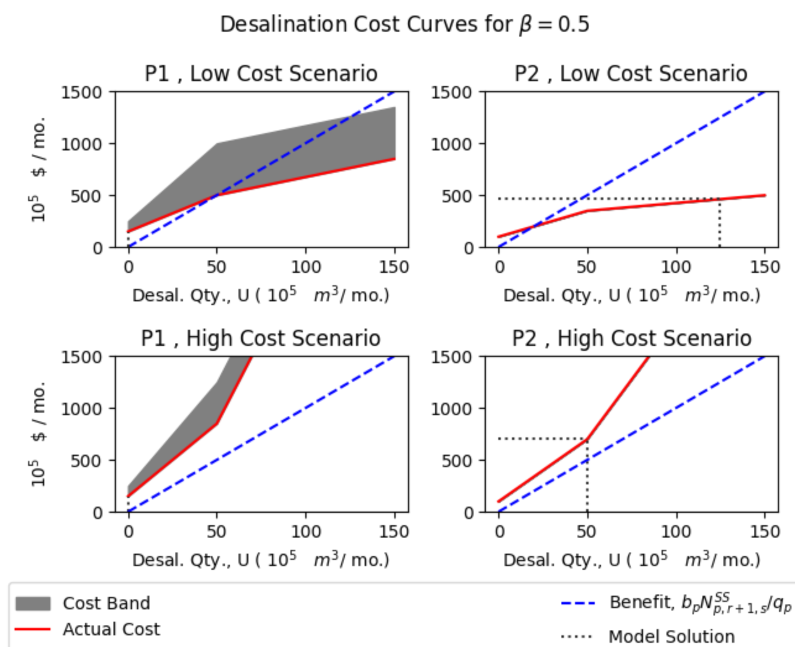


(b) Social learning and cost curves for the final model

Figure 4.8: Desalination quantity and cost relationships for the final model ($\beta_p = 0.1$)



(a) Resource usage in the final model



(b) Social learning and cost curves for the final model

Figure 4.9: Desalination quantity and cost relationships for the final model ($\beta_p = 0.5$)

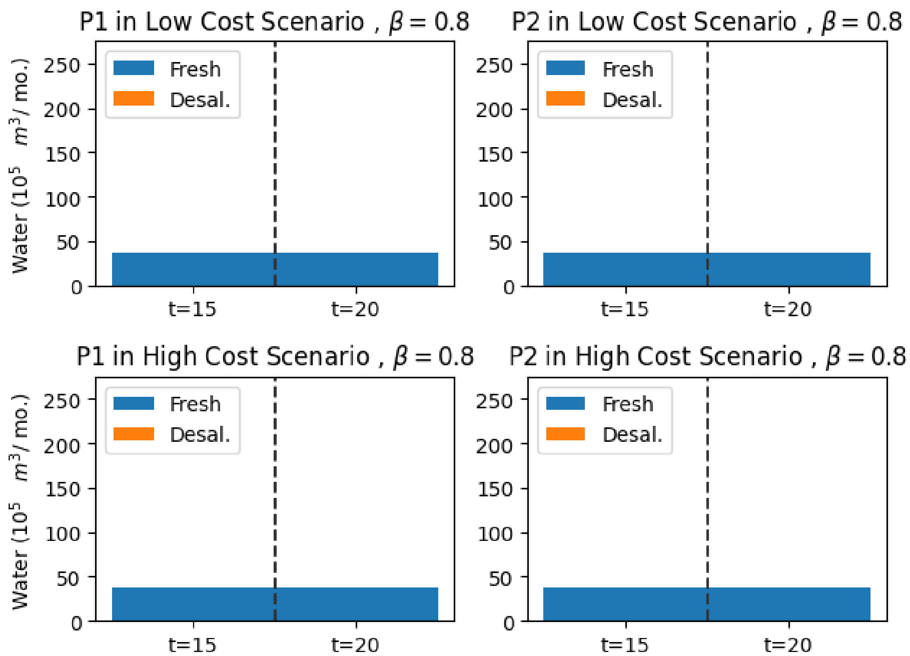


Figure 4.10: Resource usage in the final model

vantages. On the other hand, a risk-averse stance emphasizes the uncertainty inherent to technological complexity. This perspective suggests that sustainability transitions should promote equity over technology and economic growth.

These conclusions may or may not generalize to sustainability issues beyond water-resource systems. In energy systems, the externalities of greenhouse gas emissions may create ambiguity between resource availability and sustainability transitions. In other systems, such as supply chains, technological complexity may not be easily represented as latent variables.

Regardless of the specifics, the power of this approach is to allow the consideration of intermediate values of risk. A highly conservative approach to the future is one where equity is high and risks are low, but overall prosperity is also limited. The risks could be worth it though. Similarly, a risk-tolerant approach does not always produce mutually-beneficial outcomes, either. Alternatively strategies related to managing scarcity and abundance jointly enable the risks of technological failure to be controlled without being defeatist as to the future prospects of technology.

Sensitivity analysis on other parameters besides risk aversion could be performed to alter the interpretation of these conclusions. For instance, decision-makers who have past experience with desalination may perceive the R&D uncertainty differently than those without experience. This could lead two distinct decision-makers to very different investment decisions even with the same risk aversion preferences. Additionally, valuing population growth highly could increase the likelihood of investing in desalination and could be interpreted as risk-seeking behavior. For example, a speculative land developer could be modeled in this way.

One future research direction could be to simulate the bi-level optimization problem over multiple rolls of the rolling horizon. Subsequent rolls would require the development of updating rules to carry over population levels, resource reserves, and R&D outcomes from one roll to the next. A potential outcome of such research could be to understand if limited foresight likely results in long-run population growth or decline. Another outcome is to understand how a policymaker might equitably manage such long-term population changes.

Another research direction could consider multiple forms of interaction among the players and earth system boundaries. For example, the players could also interact in a market to buy or sell rights to natural resources. Secondly, multiple ESBs and natural resources could be considered in the same problem. For instance, the high energy consumption levels of desalination could be related to both the climate and water ESBs.

Last, A third research direction could consider different cost and benefit structures. For instance, a three-segment cost curve for technology could model more nuanced resource-consumption levels. For the desalination case study, brine management costs could be modeled endogenously.

Consistent with the empirical work referenced in Section 4.5, these costs would likely require non-convex terms related to process-variable interactions. Additionally, piecewise benefit curves could be added to show increasing or diminishing returns to population growth.

Chapter 5: Conclusions and Future Work

This dissertation emphasizes the relationships between socio-economic interactions and physical characteristics of water-resource systems. In Chapters 2 - 4, several water-resource equilibrium programs were developed to explore these relationships. Each chapter addressed a specific physical characteristic common to most water-resource systems. For the OR community, these themes could serve as archetypes for future research into equilibrium programming and water-resource systems. For the water-resources community, these themes could make equilibrium programming more relevant in practice.

Some results illustrate how the physical characteristics of water-resource systems influence water policies and socio-economic norms. In Chapter 2, the appropriate market structure (i.e., General Commodity Market or Cost Sharing Market) can depend on the water-demand distribution along the river. In Chapter 3, credit market prices depended on the co-benefits among BMPs. In Chapter 4, the policymaker allocated freshwater in the short-term according to each water user's long-term potential to implement desalination. Specifically, each water user's desalination potential was related to its distance from the ocean.

Conversely, other results illustrated how policies and socio-economic norms influence the physical characteristics of water-resource systems. In Chapter 2, the water-release market enabled deferment of new water-supply infrastructure in the Duck River testbed. In Chapter 3, the water-quality credit market provided incentives for the widespread adoption of nitrogen-reducing BMPs. In Chapter 4, social learning enabled the widespread adoption of desalination technology.

Risk aversion diminishes the importance of physical characteristics in the stochastic models, which are featured in Chapters 3 and 4. In Chapter 3 specifically, Prince George's County, MD has favorable land use characteristics for efficient nitrogen reduction. However, both counties install numerous nitrogen-reducing BMPs regardless of efficiency when the exceedance probability for the extreme sediment year is small. Similarly, in Chapter 4, both players receive the same fresh water allocations regardless of their desalination costs when risk aversion is high (i.e. $\beta_p = 0.8$).

The socio-economic norms in each chapter incentivized players to interact but were not always equitable. In Chapter 2, the market structures incentivized loss-reductions but were not always mutually beneficial. In Chapter 3, the water-quality credit market equalized the marginal costs of TMDL implementation to incentivize cost-effective BMP installations. However, this incentive structure could be inequitable if one player produces more water pollution than another. In Chapter 4, freshwater allocations incentivized the adoption of desalination technology but often generated unequal payoffs and risks to the players.

Altruism is a potential future research direction to incorporate equitable decision-making into water resource systems. It is defined as the tendency to help those in a disadvantaged state even if doing so carries an individual cost [160]. For example, an altruistic upstream player could increase loss-reductions beyond an "optimal" solution to aid disadvantaged players downstream. Similarly, a stormwater-management agency could sell water-quality credits without deriving a profit. Such an approach could be altruistic if the purchasing agency is under-funded and the selling agency is well funded.

Another future research direction could use risk as a common framework to link economic and altruistic motivated decision-making. In Chapter 4, water-allocation equity increased as risk aversion increased. One could imagine a similar logic applying to the work in Chapter 2. For example, the downstream players would likely receive a greater allocation of water as risk aversion to extreme drought increases. However, the models in Chapter 2 would need to be extended into a stochastic, bi-level optimization problem as used in Chapter 4 to investigate this possibility.

Finally, future research could consider computational multi-agent models of water-resource systems. Models of this type simulate agent decisions according to many possible decision frameworks such as if-then logic, genetic algorithms, and even non-convex optimization problems. Previous research has applied computational models to groundwater management [161, 162], urban water supply, and water-quality permit trading [17].

This computational approach has certain advantages and disadvantages compared to equilibrium programming. Each player's formulation is not restricted to being a convex optimization problem as with equilibrium programming. In many cases, however, this formulation flexibility comes as the expense of lacking provably optimal decisions for each player. Additionally, the solutions (e.g., water prices) in computational models often require convergence analysis to identify equilibrium points. For example, computational models with multiple equilibria can exhibit cyclical or transient solution behavior [163].

This computational approach would be particularly helpful at improving the scalability of the work in this dissertation. For example, the players in Chapters 2 and 3, who respectively represent water utilities and local governments, serve aggregations of potentially thousands of smaller-scale players (e.g., rate payers, land owners). Building equilibrium programs at this scale would not likely be feasible or of value because of the large number of individual optimization problems involved.

Furthermore, this computational approach would also be valuable for only a few number of players. Each player no longer would be restricted to solving convex optimization problems. A non-convex modeling approach would be particularly interesting for the work in Chapter 4. Such a model could enable the process modeling of desalination more explicitly and accurately. Additionally, smooth concave cost curves for desalination could replace the piecewise linear curves.

Appendix A: Generalized Nash equilibrium models for asymmetric, non-cooperative games on line graphs

A.1 Proof of Theorem 1

Proof. In this game, r_i equals the difference between the optimal objective functions of the Generalized Nash reformulation and the original line-graph game:

$$r_i = f_i^{GN}(x_i^*, y_i^*, z_i^*, \pi) - f_i^{LG}(x_i^*) \tag{A.1}$$

Assume $r_i \geq 0 \quad \forall i \in I$. In this case, $f_i^{GN}(x_i^*, y_i^*, z_i^*, \pi) = f_i^{LG}(x_i^*) \quad \forall i \notin I^C$ using an optimality argument. Otherwise, player i would chose to be in the set I^C. Therefore, $v(I) = v(I^C) = \sum_{i \in I^C} r_i$ follows from substituting Equation (A.1) into Equation (2.4) given that $r_i = 0$ for all non-participating players. This satisfies Equation (2.5a). The premise satisfies Equation (2.5b). □

A.2 Proof of Theorem 2

Proof. First note that the KKT conditions to (2.25) are necessary due to the linearity of the constraint functions and sufficient due to the concavity of the objective function since $\beta_i > 0$.

These conditions are the following.

$$0 \leq c_i^{ops} - \alpha_i + \beta_i Q_i - lf_i \gamma_i^{loss} + \gamma_i^{flow} \perp Q_i \geq 0 \tag{A.2a}$$

$$0 \leq c_i^{cu} - \pi_i^{as} + \gamma_i^{loss} \perp L_i^R \geq 0 \tag{A.2b}$$

$$0 \leq \pi_j^{as} - \gamma_i^{flow} \perp W_{i,j}^P \geq 0, \forall j \in U_i \tag{A.2c}$$

$$0 \leq lf_i Q_i - L_i^R \perp \gamma_i^{loss} \geq 0 \tag{A.2d}$$

$$0 \leq n_i + \sum_{j \in U_i} W_{i,j}^P - r_i^{fc} - Q_i + O_{i-1}^{min} \perp \gamma_i^{flow} \geq 0 \tag{A.2e}$$

Consider a node e that is not active in the loss-reduction market. Then, the following are feasible values for the variables:

$$Q_e = 0, L_e^R = 0, W_{e,j}^P = 0, \forall j \in U_e, \gamma_e^{loss} = 0, \gamma_e^{flow} = 0, \pi_e^{as} = 0.$$

To see why, take each part of (A.2) separately. (A.2a) is feasible as long as $c_e^{ops} - \alpha_e \geq 0$, which is condition (ii) in the premise. (A.2b) holds as long as $c_e^{cu} \geq 0$ which is guaranteed since all cost coefficients are positive. Conditions (A.2c), (A.2d) and the market-clearing condition (2.26b) are automatically satisfied for the given values. Note that for $j \in U_e$, (A.2c) holds if $\pi_j^{as} > 0$ or if $\pi_j^{as} = 0$. Under (iii), and considering the definition of O_e^{min}, we see that from (2.26a) $O_e^{min} = \sum_{r=1}^{e} n_r$. Thus, in (A.2e), we need $n_e + O_{e-1}^{min} = \sum_{r=1}^{e} n_r \geq r_e^{fc}$ which is (iv).

Now consider node u which alone supplies loss reduction. As $L_u^R > 0$ this means by (A.2d) that $Q_u > 0$. $L_u^R > 0$ in (A.2b) means that $\pi_u^{as} = c_u^{cu} + \gamma_u^{loss} > 0$. This in turn implies in (2.26b) and (iii) that $W^P_{d,u} = L^R_u = lf_u Q_u > 0$ is feasible. Since $Q_u > 0$, choose $\gamma^{loss}_u = \gamma^{flow}_u = 0$ so that in (A.2a) $Q_u = \frac{\alpha_u - c^{ops}_u}{\beta_u}$ which is positive by the left-most inequality in (v). (A.2c) is true since $\forall j \in U_u$, $W^P_{u,j} = 0$, $0 = \gamma^{flow}_u \leq \pi^{as}_j = 0$. Note that since $lf_u Q_u = L^R_u$ and $\gamma^{loss}_u \geq 0$, (A.2d) is feasible. (A.2e), reduces to

$$0 < Q_u \leq \sum_{r=1}^{u} n_r - r^{fc}_u \perp \gamma^{flow}_u \geq 0$$

which is true as long as Q_u satisfies

$$0 < Q_u = \frac{\alpha_u - c^{ops}_u}{\beta_u} \leq \sum_{r=1}^{u} n_r - r^{fc}_u$$

which is valid by the right-most inequality in (v).

Lastly, consider node d, a sole downstream node in D_u, active in the loss-reduction market and receiving water purchases from node u. By construction, from (A.2c), $W^P_{d,u} > 0 \Rightarrow \gamma^{flow}_d = \pi^{as}_u > 0$, the right-most part coming from the analysis above. Now let the rest of the variables have the following values: $\gamma^{loss}_d = 0, Q_d = 0, L^R_d = 0, \pi^{as}_d = 0, \gamma^{flow}_d = \pi^{as}_u > 0, W^P_{d,j} = 0, j \neq u, W^P_{d,j} = L^R_u > 0, j = u$. With those values, note that (A.2a) is satisfied as long as $\pi^{as}_u \geq \alpha_d - c^{ops}_d$ which is guaranteed by condition (vi) and taking into account the analysis above that gave $\pi^{as}_u = c^{cu}_u + \gamma^{loss}_u = c^{cu}_u$. (A.2b) is automatically satisfied with those values since $c^{cu}_d \geq 0$. (A.2c) is satisfied since $W^P_{d,u} > 0 \Rightarrow \gamma^{flow}_d = \pi^{as}_u$. (A.2d) is automatically satisfied for the given values as is (2.26b), the latter since $W^p_{d,u} = L^R_u$ and $\pi^{as}_u > 0$. Since $\gamma^{flow}_d > 0$, and given that $W^{p}_{d,u} = L^{R}_{u} = Q_u lf_u$ the last condition, (A.2e) is satisfied as long as:

$$Q_d = \sum_{r=1}^{d} n_r - r^{fc}_{d} + \left(\frac{\alpha_u - c^{ops}_{u}}{\beta_u}\right) lf_u$$

which is guaranteed by (vii).

□

A.3 Proof of Theorem 3

Proof. Consider a node $j \in U^{+}_{i,t}$. Since $W^{P}_{i,j,t} > 0$ it follows by complementarity that $\pi^{as}_{j,t} = \frac{\gamma^{flow}_{i,t}}{d_t}$. As this is true $\forall j \in U^{+}_{i,t}$ we see that the corresponding prices $\pi^{as}_{j,t}$ must be equal with $\pi_{i,t} = \frac{\gamma^{flow}_{i,t}}{d_t}$. □

A.4 Proof of Theorem 4

Proof. Consider a node i for which $L^{R}_{i,c,t} > 0$, for some $c \in C, t \in T$. Then, by (A.3e),

$$\pi^{as}_{i,t} = \frac{\sum_{t'=t}^{|T|} \gamma^{loss}_{i,c,t}}{d_t} + c^{cu}_{i,c,t}$$

Since $k \in D^{+}_{i}$, then by (A.3f), $W^{P}_{k,i,t} > 0$, we see that

$$\pi^{as}_{i,t} = \frac{\gamma^{flow}_{k,t}}{d_t}, \forall k \in D^{+}_{i}$$

□

A.5 LCP for the GCM Formulation

$$0 \leq \sum_{t'=t}^{|T|} \lambda_{i,t'}^{sup} - \sum_{t'=t}^{|T|} \sum_{c=1}^{|C|} lf_{i,c,t} \gamma_{i,c,t'}^{loss} \perp W_{i,t}^{D} \geq 0 \quad \forall t \tag{A.3a}$$

$$0 \leq d_t(c_{i,t}^{sr} - \pi_{i,t}^{as}) - \gamma_{i,t}^{flow} + \gamma_{i,t}^{cap} \perp W_{i,t}^{S} \geq 0 \quad \forall t \tag{A.3b}$$

$$0 \leq d_t(c_{i,t}^{ops} - \theta_{i,t}(Q_{i,t})) - \lambda_{i,t}^{sup} + \gamma_{i,t}^{flow} \perp Q_{i,t} \geq 0 \quad \forall t \tag{A.3c}$$

$$0 \leq d_t c_{i,t}^{cap} - \gamma_{i,t}^{cap} + \lambda_{i,t}^{aug} \perp K_{i,t} \geq 0 \quad \forall t \tag{A.3d}$$

$$0 \leq d_t(c_{i,c,t}^{cu} - \pi_{i,t}^{as}) + \sum_{t'=t}^{|T|} \gamma_{i,c,t'}^{loss} \perp L_{i,c,t}^{R} \geq 0 \quad \forall c, t \tag{A.3e}$$

$$0 \leq \delta_{us_{j,i}}^{all}(d_t \pi_{j,t}^{as} - \gamma_{i,t}^{flow}) \perp W_{i,j,t}^{P} \geq 0 \quad \forall j, t \quad , \quad j \neq i \tag{A.3f}$$

$$0 \leq \sum_{t'=1}^{t} lf_{i,c,t'} W_{i,t'}^{D} - L_{i,c,t'}^{R} \perp \gamma_{i,c,t}^{loss} \geq 0 \quad \forall c, t \tag{A.3g}$$

$$0 \leq n_i + W_{i,t}^{S} + \sum_{j=1}^{|I|} \delta_{us_{j,i}}^{all} W_{i,j,t}^{P} - r_{i,t}^{fc} + O_{i-1,t}^{min} - Q_{i,t} \perp \gamma_{i,t}^{flow} \geq 0 \quad \forall t \tag{A.3h}$$

$$0 \leq K_{i,t} - W_{i,t}^{S} \perp \gamma_{i,t}^{cap} \geq 0 \quad \forall t \tag{A.3i}$$

$$\sum_{t'=1}^{t} W_{i,t'}^{D} - Q_{i,t} = 0 \quad , \quad \lambda_{i,t}^{sup} \quad free \quad \forall t \tag{A.3j}$$

$$K_{i,t} - a_{i,t}^{req} = 0 \quad , \quad \lambda_{i,t}^{aug} \quad free \quad \forall t \tag{A.3k}$$

$$O_{i,t}^{min} = n_i - \sum_{c=1}^{|C|} \sum_{t'=1}^{t} lf_{i,c,t'} W_{i,t'}^{D} + \sum_{c=1}^{|C|} \sum_{t'=1}^{t-1} L_{i,c,t'}^{R} + O_{i-1,t}^{min} \quad \forall i, t \tag{A.3l}$$

$$\sum_{k=1}^{|I|} \delta_{ds_{k,i}}^{all} W_{k,i,t}^{P} \leq \sum_{c \in C} L_{i,c,t}^{R} + W_{i,t}^{S} \perp \pi_{i,t}^{as} \geq 0, \forall t \tag{A.3m}$$

$$\theta_{i,t}(Q_{i,t}) = \alpha_{i,t} - \beta_{i,t}Q_{i,t} \quad \forall t \tag{A.3n}$$

The endogenous functions were substituted into Equation (2.6a) prior to solving for the KKT conditions.

A.6 LCP for the CSM Formulation

$$0 \leq \sum_{t'=t}^{|T|} \lambda_{i,t'}^{sup} - \sum_{t'=t}^{|T|} \sum_{c=1}^{|C|} lf_{i,c,t}\gamma_{i,c,t'}^{loss} \perp W_{i,t}^{D} \geq 0 \quad \forall t \tag{A.4a}$$

$$0 \leq d_t(c_{i,t}^{sr} - \sum_{k=1}^{|I|} \pi_{k,t}^{as}\delta_{ds_{k,i}}^{all}) - \gamma_{i,t}^{flow} + \gamma_{i,t}^{cap} \perp W_{i,t}^{S} \geq 0 \quad \forall t \tag{A.4b}$$

$$0 \leq d_t(c_{i,t}^{ops} - \theta_{i,t}(Q_{i,t})) - \lambda_{i,t}^{sup} + \gamma_{i,t}^{flow} \perp Q_{i,t} \geq 0 \quad \forall t \tag{A.4c}$$

$$0 \leq d_t c_{i,t}^{cap} - \gamma_{i,t}^{cap} + \lambda_{i,t}^{aug} \perp K_{i,t} \geq 0 \quad \forall t \tag{A.4d}$$

$$0 \leq d_t(c_{i,c,t}^{cu} - \sum_{k=1}^{|I|} \pi_{k,t}^{as}\delta_{ds_{k,i}}^{all}) + \sum_{t'=t}^{|T|} \gamma_{i,c,t'}^{loss} \perp L_{i,c,t}^{R} \geq 0 \quad \forall c,t \tag{A.4e}$$

$$0 \leq d_t\pi_{i,t}^{as} - \gamma_{i,t}^{flow} \perp W_{i,t}^{P} \geq 0 \quad \forall t \tag{A.4f}$$

$$0 \leq \sum_{t'=1}^{t} lf_{i,c,t'}W_{i,t'}^{D} - L_{i,c,t'}^{R} \perp \gamma_{i,c,t}^{loss} \geq 0 \quad \forall c,t \tag{A.4g}$$

$$0 \leq n_i + W_{i,t}^{S} + W_{i,t}^{P} - r_{i,t}^{fc} + O_{i-1,t}^{min} - Q_{i,t} \perp \gamma_{i,t}^{flow} \geq 0 \quad \forall t \tag{A.4h}$$

$$0 \leq K_{i,t} - W_{i,t}^{S} \perp \gamma_{i,t}^{cap} \geq 0 \quad \forall t \tag{A.4i}$$

$$\sum_{t'=1}^{t} W_{i,t'}^{D} - Q_{i,t} = 0 \quad , \quad \lambda_{i,t}^{sup} \quad free \quad \forall t \tag{A.4j}$$

$$K_{i,t} - a_{i,t}^{req} = 0 \quad , \quad \lambda_{i,t}^{aug} \quad free \quad \forall t \tag{A.4k}$$

$$O^{min}_{i,t} = n_i - \sum_{c=1}^{|C|}\sum_{t'=1}^{t} lf_{i,c,t'} W^D_{i,t'} + \sum_{c=1}^{|C|}\sum_{t'=1}^{t-1} L^R_{i,c,t'} + O^{min}_{i-1,t} \quad \forall t \tag{A.4l}$$

$$\sum_{j=1}^{|I|} \delta^{all}_{us_{j,i}} (\sum_{c=1}^{|C|} L^R_{j,c,t} + W^S_{j,t}) - W^P_{i,t} \geq 0 \perp \pi^{as}_{i,t} \geq 0 \quad \forall t \tag{A.4m}$$

$$\theta_{i,t}(Q_{i,t}) = \alpha_{i,t} - \beta_{i,t} Q_{i,t} \quad \forall t \tag{A.4n}$$

The endogenous functions were substituted into Equation (2.6a) prior to solving for the KKT conditions.

A.7 LCP for the No-Market Formulation

$$0 \leq \sum_{t'=t}^{|T|} \lambda^{sup}_{i,t'} \perp W^D_{i,t} \geq 0 \quad \forall t \tag{A.5a}$$

$$0 \leq d_t c^{sr}_{i,t} - \gamma^{flow}_{i,t} + \gamma^{cap}_{i,t} \perp W^S_{i,t} \geq 0 \quad \forall t \tag{A.5b}$$

$$0 \leq d_t(c^{ops}_{i,t} - \theta_{i,t}(Q_{i,t})) - \lambda^{sup}_{i,t} + \gamma^{flow}_{i,t} \perp Q_{i,t} \geq 0 \quad \forall t \tag{A.5c}$$

$$0 \leq d_t c^{cap}_{i,t} - \gamma^{cap}_{i,t} + \lambda^{aug}_{i,t} \perp K_{i,t} \geq 0 \quad \forall t \tag{A.5d}$$

$$0 \leq n_i + W^S_{i,t} - r^{fc}_{i,t} + O^{min}_{i-1,t} - Q_{i,t} \perp \gamma^{flow}_{i,t} \geq 0 \quad \forall t \tag{A.5e}$$

$$0 \leq K_{i,t} - W^S_{i,t} \perp \gamma^{cap}_{i,t} \geq 0 \quad \forall t \tag{A.5f}$$

$$\sum_{t'=1}^{t} W^D_{i,t'} - Q_{i,t} = 0 \quad , \quad \lambda^{sup}_{i,t} \quad free \quad \forall t \tag{A.5g}$$

$$K_{i,t} - a^{req}_{i,t} = 0 \quad , \quad \lambda^{aug}_{i,t} \quad free \quad \forall t \tag{A.5h}$$

$$O_{i,t}^{min} = n_i - \sum_{c=1}^{|C|} \sum_{t'=1}^{t} lf_{i,c,t'} W_{i,t'}^{D} + O_{i-1,t}^{min} \quad \forall t \tag{A.5i}$$

$$\theta_{i,t}(Q_{i,t}) = \alpha_{i,t} - \beta_{i,t} Q_{i,t} \quad \forall t \tag{A.5j}$$

Appendix B: Reducing Pollution in River Systems using a Stochastic, Game-Theoretic Modeling Approach

B.1 Sets

- $p \in P$: players responsible for meeting TMDLs via the control of pollutants. These could include municipal pollution-control agencies (e.g., MS4s), agricultural producers, mining companies, etc.

- $w, w' \in W$: sub-watersheds within the overall watershed. This set captures the data resolution of the hydrological system (e.g., drainage areas to creeks or streams that contribute to the main river)

- $l, l' \in L$: land-use category (e.g., agricultural, urban landscaping, paved areas, open areas, forest, etc.)

- $t, t' \in T$: BMP technology type (e.g., rain garden, pervious pavement, etc.)

- $c \in C$: water quality constituent of concern for TMDL (e.g., nitrogen, phosphorus, sediment, etc.)

- $j, k \in T \times W \times L$: multi-dimensional indices equal to the Cartesian product of T, W, and L. The sole purpose of these sets is to simplify notation.

B.2 Variables

- $I_{p,t,w,l}$: Player p's BMP investment level in technologies of type t that are sited in subwatershed w and land use l ($)
- $K_{p,c}$: Credits for water quality improvements that player p purchases (positive) or sells (negative) (metric tons/year)
- $\sigma^2_{p,c}$: Function in the stochastic model representing a collection of random-variable variance and covariance terms. It is adopted solely for notational simplicity.
- $\gamma^{min}_{p,c}$: player p's dual variable for the minimum required pollution reduction requirements ($/metric ton/year)
- $\gamma^{up}_{p,t,w,l}$: player p's dual variable for the constraint that represents the upper bound on investments (dimensionless)
- π_c : price for constituent c water quality credit ($/metric ton/year)

B.3 Parameters

- $\hat{s}_{p,c,t,w,l}$: player p's benefit ratio for constituent c using investment technology t in subwatershed w and land use l. It is the amount of pollutants reduced per dollar spent. (metric tons/year/$)
- $\hat{o}^{init}_{p,c}$: player p's initial loading (i.e., outflow) for constituent c without any new BMP investments. These parameters are typically generated as an output of a water-quality model. (metric tons / year)

- $i^{up}_{p,t,w,l}$: player p's upper bound on water quality investment technology t in sub-watershed w and land use l. It represents the total amount of money that can be invested in a particular type of BMP in a particular location. ($)

- $o^{allw}_{p,c}$: player p's allowable loading (i.e., outflow) for constituent c given their TMDL allocation. These parameters are typically derived from regulatory requirements. (metric tons / year)

- $\alpha_{p,c}$: Reliability level represented as the probability of satisfying pollution reduction requirements within a particular year. (%)

These primary model parameters depend on a number of intermediate parameters originating from simulation studies, engineering judgement, and stakeholder preferences [61]:

- $a^{land}_{p,w,l}$: player p's area of land in sub-watershed w and land use type l (hectares)

- $c^{site}_{p,t,w,l}$: player p's marginal cost per unit area to install BMP technology t in sub-watershed w and land use l. It equals the present worth of the overall site costs for technology t in land use type l divided by the typical area for the BMP [77]. ($/hectare)

- $\hat{e}_{p,c,w,l}$: initial-loading export coefficients for player p. They represent the annual amount of constituent c generated per unit area in sub-watershed w and land use l. These parameters are typically generated as an output of a water-quality model. (metric tons/year/hectare)

- $\hat{r}_{p,c,t,w,l}$: reduced-loading export coefficients for player p. They represent the augmentation of initial-loading export coefficient, $\hat{e}_{p,c,w,l}$, with treatment technology t.

- $f_{p,t,w,l}$: largest fraction of land area that Player p can treat using technology t in sub-watershed w and land use l (%)

B.4 Clarifying Example for Deterministic Equivalent

Consider three investments such that $j, k \in \{1, 2, 3\}$. In this setting, Equation (3.12) expands as follows:

$$V_{p,c} = \begin{bmatrix} V_{p,c}^{s^2} & V_{p,c}^{so} \\ & \\ V_{p,c}^{so^T} & v_{p,c}^{o^2} \end{bmatrix} = \begin{bmatrix} v_{p,c,1,1}^{s^2} & v_{p,c,1,2}^{s^2} & v_{p,c,1,3}^{s^2} & v_{p,c,1}^{so} \\ v_{p,c,2,1}^{s^2} & v_{p,c,2,2}^{s^2} & v_{p,c,2,3}^{s^2} & v_{p,c,2}^{so} \\ v_{p,c,3,1}^{s^2} & v_{p,c,3,2}^{s^2} & v_{p,c,3,3}^{s^2} & v_{p,c,3}^{so} \\ v_{p,c,1}^{so} & v_{p,c,2}^{so} & v_{p,c,3}^{so} & v_{p,c}^{o^2} \end{bmatrix} \tag{B.1}$$

The scalar term $\sigma_{p,c}^2$ is calculated using the product expansion from Expression (3.7):

$$\begin{aligned} \sigma_{p,c}^2 = \begin{bmatrix} I_{p,1} \\ I_{p,2} \\ I_{p,3} \\ -1 \end{bmatrix}^T V_{p,c} \begin{bmatrix} I_{p,1} \\ I_{p,2} \\ I_{p,3} \\ -1 \end{bmatrix} &= \begin{bmatrix} v_{p,c,1,1}^{s^2} I_{p,1} + v_{p,c,2,1}^{s^2} I_{p,2} + v_{p,c,3,1}^{s^2} I_{p,3} - v_{p,c,1}^{so} \\ v_{p,c,1,2}^{s^2} I_{p,1} + v_{p,c,2,2}^{s^2} I_{p,2} + v_{p,c,3,2}^{s^2} I_{p,3} - v_{p,c,2}^{so} \\ v_{p,c,1,3}^{s^2} I_{p,1} + v_{p,c,2,3}^{s^2} I_{p,2} + v_{p,c,3,3}^{s^2} I_{p,3} - v_{p,c,3}^{so} \\ v_{p,c,1}^{so} I_{p,1} + v_{p,c,2}^{so} I_{p,2} + v_{p,c,3}^{so} I_{p,3} - v_{p,c}^{o^2} \end{bmatrix}^T \times \begin{bmatrix} I_{p,1} \\ I_{p,2} \\ I_{p,3} \\ -1 \end{bmatrix} \\ &= v_{p,c,1,1}^{s^2} I_{p,1}^2 + v_{p,c,2,1}^{s^2} I_{p,2} I_{p,1} + v_{p,c,3,1}^{s^2} I_{p,3} I_{p,1} - v_{p,1}^{so} I_{p,1} + v_{p,c,1,2}^{s^2} I_{p,1} I_{p,2} \\ &+ v_{p,c,2,2}^{s^2} I_{p,2}^2 + v_{p,c,3,2}^{s^2} I_{p,3} I_{p,2} - v_{p,c,2}^{so} I_{p,2} + v_{p,c,1,3}^{s^2} I_{p,1} I_{p,3} + v_{p,c,2,3}^{s^2} I_{p,2} I_{p,3} \\ &+ v_{p,c,3,3}^{s^2} I_{p,3}^2 - v_{p,c,3}^{so} I_{p,3} - v_{p,c,1}^{so} I_{p,1} - v_{p,c,2}^{so} I_{p,2} - v_{p,c,3}^{so} I_{p,3} + v_{p,c}^{o^2} \end{aligned} \tag{B.2}$$

Given this product expansion in Equation (B.2), $\sigma^2_{p,c}$ can be re-expressed using summation notation to recover the form of Equation (3.13c):

$$\sigma^2_{p,c} = \sum_{j=1}^{3}\sum_{k=1}^{3} v^{s^2}_{p,c,j,k} I_{p,j} I_{p,k} - 2\sum_{j=1}^{3} v^{so}_{p,j} I_{p,j} + v^{o^2}_{p,c} \tag{B.3}$$

Equation (B.2) can also be used to calculate the gradient of $\sqrt{\sigma^2_{p,c}}$, which is needed in the calculations for Expression (3.14a):

$$\begin{aligned}
&\nabla\sqrt{\sigma^2_{p,c}} \\
&= \frac{1}{2\sqrt{\sigma^2_{p,c}}} \begin{bmatrix} 2v^{s^2}_{p,c,1,1} I_{p,1} + v^{s^2}_{p,c,2,1} I_{p,2} + v^{s^2}_{p,c,3,1} I_{p,3} - v^{so}_{p,c,1} + v^{s^2}_{p,c,1,2} I_{p,2} + v^{s^2}_{p,c,1,3} I_{p,3} - v^{so}_{p,c,1} \\ v^{s^2}_{p,c,2,1} I_{p,1} + v^{s^2}_{p,c,1,2} I_{p,1} + 2v^{s^2}_{p,c,2,2} I_{p,2} + v^{s^2}_{p,c,3,2} I_{p,3} - v^{so}_{p,c,2} + v^{s^2}_{p,c,2,3} I_{p,3} - v^{so}_{p,c,2} \\ v^{s^2}_{p,c,3,1} I_{p,1} + v^{s^2}_{p,c,3,2} I_{p,2} + v^{s^2}_{p,c,1,3} I_{p,1} + v^{s^2}_{p,c,2,3} I_{p,2} + 2v^{s^2}_{p,c,3,3} I_{p,3} - 2v^{so}_{p,c,3} \end{bmatrix} \\
&= \frac{1}{2\sqrt{\sigma^2_{p,c}}} \begin{bmatrix} 2v^{s^2}_{p,c,1,1} I_{p,1} - 2v^{so}_{p,c,1} + v^{s^2}_{p,c,1,2} I_{p,2} + v^{s^2}_{p,c,1,3} I_{p,3} + v^{s^2}_{p,c,2,1} I_{p,2} + v^{s^2}_{p,c,3,1} I_{p,3} \\ 2v^{s^2}_{p,c,2,2} I_{p,2} - 2v^{so}_{p,c,2} + v^{s^2}_{p,c,1,2} I_{p,1} + v^{s^2}_{p,c,2,1} I_{p,1} + v^{s^2}_{p,c,2,3} I_{p,3} + v^{s^2}_{p,c,3,2} I_{p,3} \\ 2v^{s^2}_{p,c,3,3} I_{p,3} - 2v^{so}_{p,c,3} + v^{s^2}_{p,c,1,3} I_{p,1} + v^{s^2}_{p,c,2,3} I_{p,2} + v^{s^2}_{p,c,3,1} I_{p,1} + v^{s^2}_{p,c,3,2} I_{p,2} \end{bmatrix} \\
&= \frac{1}{\sqrt{\sigma^2_{p,c}}} \begin{bmatrix} v^{s^2}_{p,c,1,1} I_{p,1} - v^{so}_{p,c,1} + v^{s^2}_{p,c,1,2} I_{p,2} + v^{s^2}_{p,c,1,3} I_{p,3} \\ v^{s^2}_{p,c,2,2} I_{p,2} - v^{so}_{p,c,2} + v^{s^2}_{p,c,2,1} I_{p,1} + v^{s^2}_{p,c,2,3} I_{p,3} \\ v^{s^2}_{p,c,3,3} I_{p,3} - v^{so}_{p,c,3} + v^{s^2}_{p,c,3,1} I_{p,1} + v^{s^2}_{p,c,3,2} I_{p,2} \end{bmatrix}
\end{aligned} \tag{B.4}$$

Given the gradient in Equation (B.4), each component of this gradient can be re-expressed using summation notation to recover the form present in Expression (3.14a):

$$\nabla\sqrt{\sigma^2_{p,c}} = \frac{1}{\sqrt{\sigma^2_{p,c}}} \left[v^{s^2}_{p,c,j,j} I_{p,j} - v^{so}_{p,c,j} + \sum_{k\neq j} v^{s^2}_{p,c,j,k} I_{p,k} \right] \quad \forall j \in \{1,2,3\} \tag{B.5}$$

Appendix C: Understanding the Role of Technological Complexity in Water-Resource Transitions using Stochastic, Bi-level Optimization

C.1 Sub-Model 4.1

C.1.1 Input Data

Table C.1: Input data for Sub-Model 4.1

	Player(s)	Planning Years(s)	Value
b_p	1		10
c_p^f	1		1
c_p^e	1		3
$d_{p,t}$	1	0	1
		5	0.67
		10	0.44
		15	0.30
		20	0.20
		25	0.13
g_p	1		2
q_p	1		1
n_p^i	1		15
l			75
a^i			35

C.2 Sub-Model 4.2

C.2.1 Input Data

Table C.2: Input data for Sub-Model 4.2

	Player(s)	Scenarios(s)	Planning Years(s)	Value
b_p	1			10
c_p^f	1			1
c_p^e	1			100
$d_{p,t}$	1		20	0.9
g_p	1			2
q_p	1			1
n_p^i	1		10	37.5
l				12.5
a^i				62.5
c_p^{RD}	1			100
$\mathbb{P}_p(s)$	1	1		0.75
		2		0.25
α_p	1			0.8
β_p	1			Varies
i_p^B	1			50
i_p^C	1			150
c_p^A	1			100
$c_{p,s}^B$	1	1		350
		2		700
$c_{p,s}^C$	1	1		500
		2		3000

C.3 Sub-Model 4.3

C.3.1 Full Formulation

$$0 \le q_p\gamma^{dem1}_{p,r} + \gamma^{max1}_{p,r} + \sum_{s\in S}(\gamma^{min2}_{p,r+1,s} - g_p\gamma^{max2}_{p,r+1,s}) - b_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) - \gamma^{min1}_{p,r} \perp N^{FS}_{p,r} \ge 0 \quad \text{(C.1a)}$$

$$0 \le q_p\gamma^{dem2}_{p,r+1,s} + \gamma^{max2}_{p,r+1,s} - \gamma^{min2}_{p,r+1,s} - d_{p,r+1}b_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) \perp N^{SS}_{p,r+1,s} \ge 0 \quad \forall s \in S \quad \text{(C.1b)}$$

$$0 \le c^e_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) - \gamma^{min1}_{p,r} \perp E^{FS}_{p,r} \ge 0 \quad \text{(C.1c)}$$

$$0 \le d_{p,r+1}c^e_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \gamma^{min2}_{p,r+1,s} \perp E^{SS}_{p,r+1,s} \ge 0 \quad \forall s \in S \quad \text{(C.1d)}$$

$$0 \le c^f_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) + \lambda^{lim1}_{p,r} - \gamma^{dem1}_{p,r} \perp F^{FS}_{p,r} \ge 0 \quad \text{(C.1e)}$$

$$0 \le d_{p,r+1}c^f_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) + \lambda^{lim2}_{p,r+1,s} - \gamma^{dem2}_{p,r+1,s} \perp F^{SS}_{p,r+1,s} \ge 0 \quad \forall s \in S \quad \text{(C.1f)}$$

$$0 \le \lambda^{acc}_{p,r} - \lambda^{lim1}_{p,r} \perp W^{FS}_{p,r} \ge 0 \quad \text{(C.1g)}$$

$$0 \le \lambda^{acc}_{p,r} - \sum_{s\in S}\lambda^{lim2}_{p,r+1,s} \perp W^{SS}_{p,r+1} \ge 0 \quad \text{(C.1h)}$$

$$0 \le \lambda^{u}_{p,s} - \gamma^{dem2}_{p,r+1,s} \perp U_{p,s} \ge 0 \quad \forall s \in S \quad \text{(C.1i)}$$

$$0 \leq \frac{\beta_p \mathbb{P}_p(s)}{1-\alpha_p} - \gamma^{rsk}_{p,s} \perp V_{p,s} \geq 0 \quad \forall s \in S \tag{C.1j}$$

$$\sum_{s \in S} \gamma^{rsk}_{p,s} - \beta_p = 0 \quad , \quad Z_p \quad free \tag{C.1k}$$

$$0 \leq \gamma^{A}_{p,s} + \lambda^{rd}_{p,s} + c^{A}_{p} \lambda^{pw}_{p,s} - i^{A}_{p} \lambda^{u}_{p,s} \perp Y^{A}_{p,s} \geq 0 \quad \forall s \in S \tag{C.1l}$$

$$0 \leq \gamma^{B}_{p,s} + \lambda^{rd}_{p,s} + c^{B}_{p,s} \lambda^{pw}_{p,s} - i^{B}_{p} \lambda^{u}_{p,s} \perp Y^{B}_{p,s} \geq 0 \quad \forall s \in S \tag{C.1m}$$

$$0 \leq \gamma^{C}_{p,s} + \lambda^{rd}_{p,s} + c^{C}_{p,s} \lambda^{pw}_{p,s} - i^{C}_{p} \lambda^{u}_{p,s} \perp Y^{C}_{p,s} \geq 0 \quad \forall s \in S \tag{C.1n}$$

$$d_{p,r+1}(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \lambda^{pw}_{p,s} = 0 \quad , \quad c^{u}_{p,s} \quad free \quad \forall s \in S \tag{C.1o}$$

$$\begin{split} 0 \leq V_{p,s} - Z_p + \Big(& b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p + \\ & d_{p,r+1} \Big(b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s}) \Big) \Big) \perp \gamma^{rsk}_{p,s} \geq 0 \quad \forall s \in S \end{split} \tag{C.2a}$$

$$0 \leq F^{FS}_{p,r} - q_p N^{FS}_{p,r} \perp \gamma^{dem1}_{p,r} \geq 0 \tag{C.2b}$$

$$0 \leq F^{SS}_{p,r+1,s} + U_{p,s} - q_p N^{SS}_{p,r+1,s} \perp \gamma^{dem2}_{p,r+1,s} \geq 0 \quad \forall s \in S \tag{C.2c}$$

$$\sum_{p' \in P} F^{FS}_{p',r} + H^{FS}_{r} = l + \sum_{p' \in P} W^{FS}_{p',r} \quad , \quad \lambda^{lim1}_{p,r} \quad free \tag{C.2d}$$

$$\sum_{p' \in P} F^{SS}_{p',r+1,s} + H^{SS}_{r+1,s} = l + \sum_{p' \in P} W^{SS}_{p',r+1} \quad , \quad \lambda^{lim2}_{p,r+1,s} \quad free \quad \forall s \in S \tag{C.2e}$$

$$\sum_{p' \in P} W^{SS}_{p',r+1,s} = a^i - \sum_{p' \in P} W^{FS}_{p',r} \quad , \quad \lambda^{acc}_{p,r} \quad free \tag{C.2f}$$

$$0 \leq g_p n^i_p - N^{FS}_{p,r} \perp \gamma^{max1}_{p,r} \geq 0 \tag{C.2g}$$

$$0 \leq g_p N_{p,r}^{FS} - N_{p,r+1,s}^{SS} \perp \gamma_{p,r+1,s}^{max2} \geq 0 \quad \forall s \in S \tag{C.2h}$$

$$0 \leq N_{p,r}^{FS} + E_{p,r}^{FS} - n_p^i \perp \gamma_{p,r}^{min1} \geq 0 \tag{C.2i}$$

$$0 \leq N_{p,r+1,s}^{SS} + E_{p,r+1,s}^{SS} - N_{p,r}^{FS} \perp \gamma_{p,r+1,s}^{min2} \geq 0 \quad \forall s \in S \tag{C.2j}$$

$$c_{p,s}^u(U_{p,s}) = c_p^A Y_{p,s}^A + c_{p,s}^B Y_{p,s}^B + c_{p,s}^C Y_{p,s}^C - c_p^{RD} X_p^{RD} \quad , \quad \lambda_{p,s}^{pw} \quad free \quad \forall s \in S \tag{C.2k}$$

$$U_{p,s} = i_p^A Y_{p,s}^A + i_p^B Y_{p,s}^B + i_p^C Y_{p,s}^C \quad , \quad \lambda_{p,s}^u \quad free \quad \forall s \in S \tag{C.2l}$$

$$0 \leq X_{p,s}^A - Y_{p,s}^A \perp \gamma_{p,s}^A \geq 0 \quad \forall s \in S \tag{C.2m}$$

$$0 \leq X_{p,s}^A + X_{p,s}^B - Y_{p,s}^B \perp \gamma_{p,s}^B \geq 0 \quad \forall s \in S \tag{C.2n}$$

$$0 \leq X_{p,s}^B - Y_{p,s}^C \perp \gamma_{p,s}^C \geq 0 \quad \forall s \in S \tag{C.2o}$$

$$Y_{p,s}^A + Y_{p,s}^B + Y_{p,s}^C = X_p^{RD} \quad , \quad \lambda_{p,s}^{rd} \quad free \quad \forall s \in S \tag{C.2p}$$

$$c_p^{RD} = c_p^A = c_p^{A'} - \Delta c_p^A \sum_{p' \in \{\mathcal{P}:p' \neq p\}} w_{p,p'} X_{p'}^{RD} \tag{C.3a}$$

$$c_{p,s}^B = c_{p,s}^{B'} - \Delta c_{p,s}^B \sum_{p' \in \{\mathcal{P}:p' \neq p\}} w_{p,p'} (Y_{p',s}^B + Y_{p',s}^C) \quad \forall s \in S \tag{C.3b}$$

$$c_{p,s}^C = c_{p,s}^B + c_{p,s}^m (i_p^C - i_p^B) \quad \forall s \in S \tag{C.3c}$$

$$0 \leq \sum_{p \in P} \lambda_{p,r}^{lim1} \perp H_r^{FS} \geq 0 \tag{C.3d}$$

$$0 \leq \sum_{p \in P} \lambda_{p,r+1,s}^{lim2} \perp H_{r+1,s}^{SS} \quad \forall s \in S \tag{C.3e}$$

$$\lambda_{p,r}^{lim1} = \sum_{p' \neq p} v_{p,p'}^{FS} \lambda_{p',r}^{lim1} \quad , \quad p < |P| \tag{C.3f}$$

$$\lambda_{p,r+1,s}^{lim2} = \sum_{p' \neq p} v_{p,p',s}^{SS} \lambda_{p'r+1,s}^{lim2} \quad , \quad p < |P| \quad , \quad s \in S \tag{C.3g}$$

$$\lambda_{p,r}^{acc} = \sum_{p' \neq p} v_{p,p'}^{A} \lambda_{p',r}^{acc} \quad , \quad p < |P| \tag{C.3h}$$

C.3.2 Input Data

Table C.3: Input data for Sub-Model 4.3

	Player(s)	Scenarios(s)	Planning Years(s)	Value
b_p	1,2			10
c_p^f	1,2			1
c_p^e	1,2			100
$d_{p,t}$	1,2		20	0.9
g_p	1,2			2
q_p	1,2			1
n_p^i	1,2		10	37.5
l				25
a^i				100
$\mathbb{P}_p(s)$	1,2	1		0.75
		2		0.25
α_p	1,2			0.8
β_p	1,2			0.1
i_p^B	1,2			50
i_p^C	1,2			150
$c_p^{A'}$	1			250
	2			100
$c_{p,s}^{B'}$	1	1		1000
		2		1250
	2	1		350
		2		700
$c_{p,s}^m$	1	1		3.5
		2		33
	2	1		1.5
		2		23
Δc_p^A	1			100
	2			0
$\Delta c_{p,s}^B$	1	1		500
		2		400
	2	1,2		0
$w_{p,2}$	1			1
$w_{p,1}$	2			1
$v_{p,2}^{FS}$	1			0.5
$v_{p,2,s}^{SS}$	1	1		$\frac{7}{3}$
		2		$\frac{33}{23}$
$v_{p,2}^A$	1			1

C.4 Final Model

C.4.1 Sets

- $p \in P$: Players utilizing natural resources for economic growth
- $t \in \mathcal{T}$: Planning period for which players make or adjust planning decisions related to population growth and resource utilization
- $s \in S$: Discrete scenarios representing technology ROI outcomes

C.4.2 Variables

C.4.2.1 Upper-Level Variables

- $L^{FS}_{p,t}$: The upper-level player's allocation of the finite resource to lower-level player p in the current planning period t (mass/month)
- W^{FS}_{t}: The upper-level player's withdrawal of the finite resource from reserve in planning period t (mass/month)
- $L^{SS}_{p,t+1,s}$: The upper-level player's allocation of the finite resource to lower-level player p in scenario s of the next planning period $t+1$ (mass/month)
- W^{SS}_{t+1}: The upper-level player's withdrawal of the finite resource from reserve in planning period $t+1$ (mass/month)
- A_{t+1}: amount of the finite-resource reserve remaining in time period $t+1$ (mass/month)

- X_p^{RD}: Binary investment decision indicating if player p pays the R&D fixed cost (dimensionless)
- $X_{p,s}^{A}$: Activation term for the first point on player p's piece-wise cost curve in scenario s (dimensionless)
- $X_{p,s}^{B}$: Activation term for the second point on player p's piece-wise cost curve in transition scenario s (dimensionless)

C.4.2.2 Lower-Level Variables

- $N_{p,t}^{FS}$: Population served by player p during planning period t (Thousands)
- $N_{p,t+1,s}^{SS}$: Population served by player p in scenario s during planning period $t+1$ (Thousands)
- $E_{p,t}^{FS}$: Population lost for player p during planning period t (Thousands)
- $E_{p,t+1,s}^{SS}$: Population lost for player p in scenario s during planning period $t+1$ (Thousands)
- $F_{p,t}^{FS}$: Player p's average monthly consumption of the finite resource during planning period t (mass/month)
- $F_{p,t+1,s}^{SS}$: Player p's average monthly consumption of the finite resource in scenario s during planning period $t+1$ (mass/month)
- $U_{p,s}$: Player p's average monthly consumption of the practically unlimited resource in scenario s (mass/month)
- $V_{p,s}$: Player p's benefit shortfall in scenario s (\$)

- Z_p : Player p's threshold payoff for experiencing shortfall ($)
- $Y^A_{p,s}$: First domain weighting term for player p's piece-wise technology cost curve in scenario s (dimensionless)
- $Y^B_{p,s}$: Second domain weighting term for player p's piece-wise technology cost curve in scenario s (dimensionless)
- $Y^C_{p,s}$: Third domain weighting term for player p's piece-wise technology cost curve in scenario s (dimensionless)
- $c^u_{p,s}$: Player p's cost to access the practically unlimited resource in scenario s ($)
- $\gamma^{rsk}_{p,s}$: Shadow price associated with the net-benefit-shortfall constraint for player p in scenario s (dimensionless)
- $\gamma^{dem1}_{p,t}$: Shadow price associated with the natural-resource-demand constraint for player p in planning period t ($/mass/mo.)
- $\gamma^{dem2}_{p,t+1,s}$: Shadow price associated with the natural-resource-demand constraint for player p in planning period $t+1$ and scenario s ($/mass/mo.)
- $\gamma^{lim1}_{p,t}$: Shadow price associated with the limit to the finite-resource for player p in planning period t ($/mass/mo.)
- $\gamma^{lim2}_{p,t+1,s}$: Shadow price associated with the limit to the finite-resource for player p in planning period $t+1$ and scenario s ($/mass/mo.)
- $\gamma^{max1}_{p,t}$: Shadow price associated with the constraint on the maximum population growth for player p in planning period t ($/thousand)

- $\gamma^{max2}_{p,t+1,s}$: Shadow price associated with the constraint on the maximum population growth for player p in planning period $t+1$ and scenario s ($/thousand)

- $\gamma^{min1}_{p,t}$: Shadow price associated with the constraint on maintaining the minimum population level for player p in planning period t ($/thousand)

- $\gamma^{min2}_{p,t+1,s}$: Shadow price associated with the constraint on maintaining the minimum population level for player p in planning period $t+1$ and scenario s ($/thousand)

- $\lambda^{pw}_{p,s}$: Shadow price associated with the definitional constraint for player p's piece-wise cost function in scenario s (dimensionless)

- $\lambda^{u}_{p,s}$: Shadow price associated with the definitional constraint for player p's utilization of the practically unlimited resource in scenario s ($/mass/month)

- $\gamma^{A}_{p,s}$: Shadow price associated with the constraint on the first domain weighting term for player p in scenario s ($)

- $\gamma^{B}_{p,s}$: Shadow price associated with the constraint on the second domain weighting term for player p in scenario s ($)

- $\gamma^{C}_{p,s}$: Shadow price associated with the constraint on the third domain weighting term for player p in scenario s ($)

- $\lambda^{rd}_{p,s}$: Shadow price associated with the constraint of $R\&D$ investment on the domain weighting terms ($)

- c^{A}_{p} : Cost at player p's first piece-wise point ($)

- $c_{p,s}^B$: Cost at player p's second piece-wise point in scenario s ($)

- $c_{p,s}^C$: Cost at player p's third piece-wise point in scenario s ($)

C.4.3 Parameters

- b_p: Benefit obtained per unit of population maintained by player p ($ / thousand / month)

- c_p^f: Player p's unit cost for the finite resource ($ / unit mass / month)

- c_p^e: Player p's cost per unit of lost population ($ / thousand)

- $d_{p,t}$: Player p's discount rate in planning period t (dimensionless)

- g_p: Population growth rate player p (dimensionless)

- q_p: Player p's resource demand per unit of population (mass / month / thousand)

- n_p^i: Player p's starting population (thousands)

- l: Extraction limit of the finite resource (mass / month)

- a^i: initial accumulation of finite resources expressed as the quantity that can be removed on average each month throughout one planning period (mass / month)

- $\mathbb{P}_p(s)$: Probability of ROI scenario s (dimensionless)

- α_p: Complement of the quantile used in the CVaR calculation for player p (dimensionless)

- β_p: Risk weighting parameter for player p (dimensionless)

- i_p^B: Second break point for player p's piece-wise cost curve (mass / month)

- i_p^C: Third break point for player p's piece-wise cost curve (mass / month)

- $c_p^{A^{'}}$: Technology cost at first piece-wise point for player p without any social learning contributions from other players ($ / month)

- $c_{p,s}^{B^{'}}$: Technology cost at second piece-wise point for player p in scenario s without any social learning contributions from other players ($ / month)

- $c_{p,s}^{m}$: Player p's marginal technology cost after reaching maturity in scenario s ($ / mass / month)

- Δc_p^A : Player p's maximum possible decrease of c_p^A given social learning contributions from other players ($)

- $\Delta c_{p,s}^B$: Player p's maximum possible decrease of $c_{p,s}^B$ given technological learning contributions from other players in scenario s ($)

- $w_{p,p'}$: Weight relating the impact of player $p^{'}$ on the social learning of player p (dimensionless)

C.4.4 SOS1 Reformulation of Program 4.8

$$\max_{L^{FS},W^{FS},L^{SS},W^{SS},A,X^{RD},X^A,X^B} \sum_{p\in P}\Big(1-\beta_p\Big)\Big(b_p N_{p,r}^{FS} - c_p^f F_{p,r}^{FS} - c_p^e E_{p,r}^{FS} - c_p^{RD} X_p^{RD} + d_{p,r+1}\sum_{s\in S}\mathbb{P}_p(s)\Big(b_p N_{p,r+1,s}^{SS} - c_p^f F_{p,r+1,s}^{SS} - c_p^e E_{p,r+1,s}^{SS} - c_{p,s}^u(U_{p,s})\Big)\Big) + \beta_p\left(Z_p - \frac{1}{1-\alpha_p}\sum_{s\in S}\mathbb{P}_p(s)V_{p,s}\right)$$

s.t.

$$q_p\gamma^{dem1}_{p,r} + \gamma^{max1}_{p,r} + \sum_{s\in S}(\gamma^{min2}_{p,r+1,s} - g_p\gamma^{max2}_{p,r+1,s}) - b_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) - \gamma^{min1}_{p,r} = K^{N1}_{p,r}$$

$$q_p\gamma^{dem2}_{p,r+1,s} + \gamma^{max2}_{p,r+1,s} - \gamma^{min2}_{p,r+1,s} - d_{p,r+1}b_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) = K^{N2}_{p,r+1,s} \quad \forall s \in S$$

$$c^e_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) - \gamma^{min1}_{p,r} = K^{E1}_{p,r}$$

$$d_{p,r+1}c^e_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \gamma^{min2}_{p,r+1,s} = K^{E2}_{p,r+1,s} \quad \forall s \in S$$

$$c^f_p((1-\beta_p) + \sum_{s\in S}\gamma^{rsk}_{p,s}) + \gamma^{lim1}_{p,r} - \gamma^{dem1}_{p,r} = K^{F1}_{p,r}$$

$$d_{p,r+1}c^f_p(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) + \gamma^{lim2}_{p,r+1,s} - \gamma^{dem2}_{p,r+1,s} = K^{F2}_{p,r+1,s} \quad \forall s \in S$$

$$\lambda^u_{p,s} - \gamma^{dem2}_{p,r+1,s} = K^U_{p,s} \quad \forall s \in S$$

$$\frac{\beta_p\mathbb{P}_p(s)}{1-\alpha_p} - \gamma^{rsk}_{p,s} = K^V_{p,s} \quad \forall s \in S$$

$$\sum_{s\in S}\gamma^{rsk}_{p,s} - \beta_p = 0 \quad , \quad Z_p \quad free$$

$$\gamma^A_{p,s} + \lambda^{rd}_{p,s} + c^A_p\lambda^{pw}_{p,s} - i^A_p\lambda^u_{p,s} = K^{Y^A}_{p,s} \quad \forall s \in S$$

$$\gamma^B_{p,s} + \lambda^{rd}_{p,s} + c^B_{p,s}\lambda^{pw}_{p,s} - i^B_p\lambda^u_{p,s} = K^{Y^B}_{p,s} \quad \forall s \in S$$

$$\gamma^C_{p,s} + \lambda^{rd}_{p,s} + c^C_{p,s}\lambda^{pw}_{p,s} - i^C_p\lambda^u_{p,s} = K^{Y^C}_{p,s} \quad \forall s \in S$$

$$d_{p,r+1}(\mathbb{P}_p(s)(1-\beta_p) + \gamma^{rsk}_{p,s}) - \lambda^{pw}_{p,s} = 0 \quad , \quad c^u_{p,s} \quad free \quad \forall s \in S$$

$$V_{p,s} - Z_p + \Big(b_p N^{FS}_{p,r} - c^f_p F^{FS}_{p,r} - c^e_p E^{FS}_{p,r} - c^{RD}_p X^{RD}_p +$$
$$d_{p,r+1}\Big(b_p N^{SS}_{p,r+1,s} - c^f_p F^{SS}_{p,r+1,s} - c^e_p E^{SS}_{p,r+1,s} - c^u_{p,s}(U_{p,s})\Big)\Big) = K^{rsk}_{p,s} \quad \forall s \in S$$

$$F^{FS}_{p,r} - q_p N^{FS}_{p,r} = K^{dem1}_{p,r}$$

$$F^{SS}_{p,r+1,s} + U_{p,s} - q_p N^{SS}_{p,r+1,s} = K^{dem2}_{p,r+1,s} \quad \forall s \in S$$

$$L^{FS}_{p,r} - F^{FS}_{p,r} = K^{lim1}_{p,r}$$

$$L^{SS}_{p,r+1,s} - F^{SS}_{p,r+1,s} = K^{lim2}_{p,r+1,s} \quad \forall s \in S$$

$$g_p n^i_p - N^{FS}_{p,r} = K^{max1}_{p,r}$$

$$g_p N^{FS}_{p,r} - N^{SS}_{p,r+1,s} = K^{max2}_{p,r+1,s} \quad \forall s \in S$$

$$N^{FS}_{p,r} + E^{FS}_{p,r} - n^i_p = K^{min1}_{p,r}$$

$$N^{SS}_{p,r+1,s} + E^{SS}_{p,r+1,s} - N^{FS}_{p,r} = K^{min2}_{p,r+1,s} \quad \forall s \in S$$

$$c^u_{p,s}(U_{p,s}) = c^A_p Y^A_{p,s} + c^B_{p,s} Y^B_{p,s} + c^C_{p,s} Y^C_{p,s} - c^{RD}_p X^{RD}_p \quad , \quad \lambda^{pw}_{p,s} \quad free \quad \forall s \in S$$

$$U_{p,s} = i^A_p Y^A_{p,s} + i^B_p Y^B_{p,s} + i^C_p Y^C_{p,s} \quad , \quad \lambda^u_{p,s} \quad free \quad \forall s \in S$$

$$X^A_{p,s} - Y^A_{p,s} = K^{\gamma^A}_{p,s} \quad \forall s \in S$$

$$X^A_{p,s} + X^B_{p,s} - Y^B_{p,s} = K^{\gamma^B}_{p,s} \quad \forall s \in S$$

$$X^B_{p,s} - Y^C_{p,s} = K^{\gamma^C}_{p,s} \quad \forall s \in S$$

$$Y_{p,s}^{A} + Y_{p,s}^{B} + Y_{p,s}^{C} = X_{p}^{RD} \quad , \quad \lambda_{p,s}^{rd} \quad free \quad \forall s \in S$$

$$I_{p,r}^{N1} + J_{p,r}^{N1} = (N_{p,r}^{FS} + K_{p,r}^{N1})/2$$

$$I_{p,r}^{N1} - J_{p,r}^{N1} = (N_{p,r}^{FS} - K_{p,r}^{N1})/2$$

$$I_{p,r+1,s}^{N2} + J_{p,r+1,s}^{N2} = (N_{p,r+1,s}^{SS} + K_{p,r+1,s}^{N2})/2 \quad \forall s \in S$$

$$I_{p,r+1,s}^{N2} - J_{p,r+1,s}^{N2} = (N_{p,r+1,s}^{SS} - K_{p,r+1,s}^{N2})/2 \quad \forall s \in S$$

$$I_{p,r}^{E1} + J_{p,r}^{E1} = (E_{p,r}^{FS} + K_{p,r}^{E1})/2$$

$$I_{p,r}^{E1} - J_{p,r}^{E1} = (E_{p,r}^{FS} - K_{p,r}^{E1})/2$$

$$I_{p,r+1,s}^{E2} + J_{p,r+1,s}^{E2} = (E_{p,r+1,s}^{SS} + K_{p,r+1,s}^{E2})/2 \quad \forall s \in S$$

$$I_{p,r+1,s}^{E2} - J_{p,r+1,s}^{E2} = (E_{p,r+1,s}^{SS} - K_{p,r+1,s}^{E2})/2 \quad \forall s \in S$$

$$I_{p,r}^{F1} + J_{p,r}^{F1} = (F_{p,r}^{FS} + K_{p,r}^{F1})/2$$

$$I_{p,r}^{F1} - J_{p,r}^{F1} = (F_{p,r}^{FS} - K_{p,r}^{F1})/2$$

$$I_{p,r+1,s}^{F2} + J_{p,r+1,s}^{F2} = (F_{p,r+1,s}^{SS} + K_{p,r+1,s}^{F2})/2 \quad \forall s \in S$$

$$I_{p,r+1,s}^{F2} - J_{p,r+1,s}^{F2} = (F_{p,r+1,s}^{SS} - K_{p,r+1,s}^{F2})/2 \quad \forall s \in S$$

$$I_{p,s}^{U} + J_{p,s}^{U} = (U_{p,s} + K_{p,s}^{U})/2 \quad \forall s \in S$$

$$I_{p,s}^{U} - J_{p,s}^{U} = (U_{p,s} - K_{p,s}^{U})/2 \quad \forall s \in S$$

$$I_{p,s}^{V} + J_{p,s}^{V} = (V_{p,s} + K_{p,s}^{V})/2 \quad \forall s \in S$$

$$I^{V}_{p,s} - J^{V}_{p,s} = (V_{p,s} - K^{V}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^A}_{p,s} + J^{Y^A}_{p,s} = (Y^{A}_{p,s} + K^{Y^A}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^A}_{p,s} - J^{Y^A}_{p,s} = (Y^{A}_{p,s} - K^{Y^A}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^A}_{p,s} + J^{Y^A}_{p,s} = (Y^{A}_{p,s} + K^{Y^A}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^B}_{p,s} - J^{Y^B}_{p,s} = (Y^{B}_{p,s} - K^{Y^B}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^C}_{p,s} + J^{Y^C}_{p,s} = (Y^{C}_{p,s} + K^{Y^C}_{p,s})/2 \quad \forall s \in S$$

$$I^{Y^C}_{p,s} - J^{Y^C}_{p,s} = (Y^{C}_{p,s} - K^{Y^C}_{p,s})/2 \quad \forall s \in S$$

$$I^{rsk}_{p,s} + J^{rsk}_{p,s} = (\gamma^{rsk}_{p,s} + K^{rsk}_{p,s})/2 \quad \forall s \in S$$

$$I^{rsk}_{p,s} - J^{rsk}_{p,s} = (\gamma^{rsk}_{p,s} - K^{rsk}_{p,s})/2 \quad \forall s \in S$$

$$I^{dem1}_{p,r} + J^{dem1}_{p,r} = (\gamma^{dem1}_{p,r} + K^{dem1}_{p,r})/2$$

$$I^{dem1}_{p,r} - J^{dem1}_{p,r} = (\gamma^{dem1}_{p,r} - K^{dem1}_{p,r})/2$$

$$I^{dem2}_{p,r+1,s} + J^{dem2}_{p,r+1,s} = (\gamma^{dem2}_{p,r+1,s} + K^{dem2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{dem2}_{p,r+1,s} - J^{dem2}_{p,r+1,s} = (\gamma^{dem2}_{p,r+1,s} - K^{dem2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{lim1}_{p,r} + J^{lim1}_{p,r} = (\gamma^{lim1}_{p,r} + K^{lim1}_{p,r})/2$$

$$I^{lim1}_{p,r} - J^{lim1}_{p,r} = (\gamma^{lim1}_{p,r} - K^{lim1}_{p,r})/2$$

$$I^{lim2}_{p,r+1,s} + J^{lim2}_{p,r+1,s} = (\gamma^{lim2}_{p,r+1,s} + K^{lim2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{lim2}_{p,r+1,s} - J^{lim2}_{p,r+1,s} = (\gamma^{lim2}_{p,r+1,s} - K^{lim2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{max1}_{p,r} + J^{max1}_{p,r} = (\gamma^{max1}_{p,r} + K^{max1}_{p,r})/2$$

$$I^{max1}_{p,r} - J^{max1}_{p,r} = (\gamma^{max1}_{p,r} - K^{max1}_{p,r})/2$$

$$I^{max2}_{p,r+1,s} + J^{max2}_{p,r+1,s} = (\gamma^{max2}_{p,r+1,s} + K^{max2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{max2}_{p,r+1,s} - J^{max2}_{p,r+1,s} = (\gamma^{max2}_{p,r+1,s} - K^{max2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{min1}_{p,r} + J^{min1}_{p,r} = (\gamma^{min1}_{p,r} + K^{min1}_{p,r})/2$$

$$I^{min1}_{p,r} - J^{min1}_{p,r} = (\gamma^{min1}_{p,r} - K^{min1}_{p,r})/2$$

$$I^{min2}_{p,r+1,s} + J^{min2}_{p,r+1,s} = (\gamma^{min2}_{p,r+1,s} + K^{min2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{min2}_{p,r+1,s} - J^{min2}_{p,r+1,s} = (\gamma^{min2}_{p,r+1,s} - K^{min2}_{p,r+1,s})/2 \quad \forall s \in S$$

$$I^{\gamma^A}_{p,s} + J^{\gamma^A}_{p,s} = (\gamma^A_{p,s} + K^{\gamma^A}_{p,s})/2 \quad \forall s \in S$$

$$I^{\gamma^A}_{p,s} - J^{\gamma^A}_{p,s} = (\gamma^A_{p,s} - K^{\gamma^A}_{p,s})/2 \quad \forall s \in S$$

$$I^{\gamma^B}_{p,s} + J^{\gamma^B}_{p,s} = (\gamma^B_{p,s} + K^{\gamma^B}_{p,s})/2 \quad \forall s \in S$$

$$I^{\gamma^B}_{p,s} - J^{\gamma^B}_{p,s} = (\gamma^B_{p,s} - K^{\gamma^B}_{p,s})/2 \quad \forall s \in S$$

$$I^{\gamma^C}_{p,s} + J^{\gamma^C}_{p,s} = (\gamma^C_{p,s} + K^{\gamma^C}_{p,s})/2 \quad \forall s \in S$$

$$I^{\gamma^C}_{p,s} - J^{\gamma^C}_{p,s} = (\gamma^C_{p,s} - K^{\gamma^C}_{p,s})/2 \quad \forall s \in S$$

$$\sum_{p\in P} L^{FS}_{p,r} = l + W^{FS}_r$$

$$\sum_{p\in P} L^{SS}_{p,r+1,s} = l + W^{SS}_{r+1} \quad \forall s \in S$$

$$A_{r+1} = a^i - W^{FS}_r$$

$$W^{SS}_{r+1} \leq A_{r+1}$$

$$X^{RD}_p \in \{0,1\}$$

$$X^A_{p,s}, X^B_{p,s} \in \{0,1\} \quad \forall s \in S$$

$$X^A_{p,s} + X^B_{p,s} = X^{RD}_p \quad \forall (p,s) \in S \times P$$

$$c^{RD}_p = c^A_p = c^{A'}_p - \Delta c^A_p \sum_{p'\in\{\mathcal{P}:p'\neq p\}} w_{p,p'} X^{RD}_{p'}$$

$$c^B_{p,s} = c^{B'}_{p,s} - \Delta c^B_{p,s} \sum_{p'\in\{\mathcal{P}:p'\neq p\}} w_{p,p'} (Y^B_{p',s} + Y^C_{p',s})$$

$$c^C_{p,s} = c^B_{p,s} + c^m_{p,s}(i^C_p - i^B_p)$$

$$L^{FS}, L^{SS}, W, A, K \geq 0$$

$$(I,J) \in SOS1$$

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