**Nonlinear Robust Optimal Design and Operation of Effluent Treatment Systems**

by

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A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science

in

PROCESS CONTROL

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# Abstract

The optimal design and operation of effluent treatment system networks poses a significant challenge in the present time, with the imposition of stricter environmental regulations and an increased demand for resources exacerbated by a diminishing resource pool. In practice, this problem presents an additional layer of complexity owing to the presence of uncertainty in the operation of the system. This uncertainty may come from a variety of sources, such as effluent flow rate, contaminant concentration, and treatment unit removal efficiency. Therefore, the need to focus on developing a stochastic optimization framework for the optimal design and operation of effluent treatment systems has been well-recognized.

Robust and stochastic optimization techniques have been explored in the literature for water network optimization under uncertainty. Robust optimization solves for the worst case of uncertainty realized and presents a conservative solution to the problem that would be valid for any realization of uncertainty it was solved for. In contrast, stochastic optimization deals with uncertainty in an optimization problem by assuming that the probability distribution of the uncertainty is known and seeks to address the uncertainty through different techniques. Uncertainty in optimization problems can be dealt with using a variety of techniques, such as scenario-based programming, chance constrained programming, and the decision rule approach. This thesis presents a study of the applicability of the decision rule approach - specifically, the affine decision rule - in dealing with uncertainty in the optimal design and operation of effluent treatment systems. The main aim of this thesis was to obtain i) robust process design, and ii) robust operational policies, that is, a set of decision rules for the operation of the effluent treatment system, which are easily applicable for any realization of uncertainty that the problem has been modeled to handle.

The thesis compared three approaches to modeling the nonlinear effluent treatment system network under uncertainty. The first approach involved the use of McCormick envelopes in developing a linear framework to which the affine decision rule formulation was applied. The second approach employed first order Taylor series approximation around the nominal process network to linearize the system, and the affine decision rule was applied to this approximated model. The third approach used two-stage nonlinear robust optimization of the model linearized around uncertainty, in which the affine decision rule formulation was applied to the control variables. The formerly intractable model was transformed into its tractable form using the affine decision rule, and the finite, robust counterpart of the problem was modeled using the property of strong duality in linear programming problems, for a defined uncertainty set. The thesis applied these three approaches to the operation of a small water treatment model [1]. The performance, advantages, and limitations of each approach were then analyzed and contrasted. The two-stage nonlinear robust optimization approach using the affine decision rule was found to offer superior performance over the other approaches, and this approach was chosen to tackle a larger optimization problem – the optimal design and operation of the effluent treatment and steam generation system network for a SAGD reservoir [2].

# Acknowledgements

Firstly, I extend my deepest gratitude to my supervisor, Dr. Zukui Li. Dr. Li - your patience and support has been a steady driving force at every stage of my graduate studies. Thank you for taking the time to guide me through a new and initially rather daunting field of study to me, and allowing me the flexibility to explore it to my interest. Furthermore, I thank you and the CME Department for maintaining a productive and encouraging research environment that has been a joy to work in. I would also like to thank NSERC, Canada for the funding received during the course of my graduate studies.

I would like to thank my research group members - Yashas, Said, Hossein, Farough, and Anjana. It has been a pleasure to work alongside you, and I thank you for your help at various stages of my studies. Every input from you has made me better at what I do, and I appreciate all the conversations we had.

I am especially grateful to the set of friends, or perhaps more aptly put, the family that I am privileged to have built here. Hareem, you have been a constant supportive presence since the very first day of university; you are instrumental in making Edmonton my home. Yashas, thank you for being a sounding board for all of my ideas, and for the many hours of brainstorming. To the both of you, and Pai, Ananthan, Alireza, Dave, Fereshteh, and many more cherished friends at DICE - all of you constituted the best office family a person could ask for; thank you for your company during each long day, and reminding me to take a break during those longer days.

A special note of thanks to my undergraduate mentor, Dr. Madakyaru, for introducing me to the world of Process Control, and being a constant support system through graduate school. I thank my parents and my sister, for sending me to Canada with all of their love, and unwavering belief in my abilities. And lastly, I would also like to thank my friends back home in India, particularly Sanober, for keeping me grounded and cheerful, one video call, one well-timed text message at a time.

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### Parameters

| | |
|---|---|
| $\beta^{bbd}$ | Steam conversion efficiency of $OTSG$ in the SAGD model |
| $\beta^{emul}$ | Bitumen emulsion separation ratio in the SAGD model |
| $a_{tu}^{fix}$ | Fixed cost slope parameters for treatment units in the SAGD model |
| $a_{tu}^{var}$ | Variable cost slope parameters for treatment units in the SAGD model |
| $b_{tu}^{fix}$ | Fixed cost intercept parameters for treatment units in the SAGD model |
| $b_{tu}^{var}$ | Variable cost intercept parameters for treatment units in the SAGD model |
| $Bound^{low}$ | Lower bound on flow (tonne/hr) in the small water treatment model |
| $C_c^{target}$ | Target concentration to be achieved in the final stream in the small water treatment model (ppm) |
| $C_{s,c}$ | Concentration of $c$ in source water $s$ (ppm) |
| $C_{sgu,c}^{target}$ | Target inlet concentration of $c$ to all steam generation units $sgu$ $s$ (ppm) in the SAGD model |
| $C_{tu,c}^{max}$ | Maximum allowable inlet concentration of $c$ to all treatment units $tu$ $s$ (ppm) in the SAGD model |
| $cost_s^{fix}$ | Fixed cost parameters for source water in the SAGD model |
| $cost_s^{var}$ | Variable cost parameters for source water in the SAGD model |

| | |
|---|---|
| $Demand^{high}$ | Higher limit of steam demand from the well injection site (tonne/hr) in the SAGD model |
| $Demand^{low}$ | Lower limit of steam demand from the well injection site (tonne/hr) in the SAGD model |
| $Demand^{steam}$ | Steam demand from the well injection site at nominal conditions (tonne/hr) in the SAGD model |
| $F_s$ | Flow rate of source water from $s$ (tonne/hr) in the small water treatment model |
| $F_s^*$ | Nominal value for source water flow (tonne/hr) in the small water treatment model |
| $F_{tu}^{loss}$ | Treatment unit flow loss from treatment units $tu$ (tonne/hr) in the SAGD model |
| $HY$ | Number of hours of operation of the plant (hr/yr) in the SAGD model |
| $NS^{max}$ | Maximum number of streams allowed into the treatment units in the SAGD model |
| $RR_{tu,c}$ | Removal ratio of $c$ in $tu$ |

**Index $\in$ Sets for the small water treatment model**

| | |
|---|---|
| $c \in C$ | Contaminants<br>$c \in \{A, B\}$<br>$A$ - Compound A<br>$B$ - Compound B |
| $s \in S$ | Water sources<br>$s \in \{s_1, s_2\}$<br>$s_1$ - Source 1<br>$s_2$ - Source 2 |
| $tu \in TU$ | Treatment units<br>$tu \in \{tu_1, tu_2\}$<br>$tu_1$ - Treatment unit 1<br>$tu_2$ - Treatment unit 2 |

**Index $\in$ Sets for the SAGD model**

| | |
|---|---|
| $c \in C$ | Contaminants<br>$c \in \{O, Si, TH, TSS\}$<br>$O$ - Oil<br>$Si$ - Si<br>$TH$ - Total Hardness<br>$TSS$ - Total Suspended Solids |
| $s \in S$ | Water sources<br>$s \in \{PW, MUW, BBD\}$<br>$PW$ - Produced Water<br>$MUW$ - Make Up Water<br>$BBD$ - Boiler Blow Down |
| $sgu \in SGU$ | Steam Generation Units<br>$sgu \in \{HRSG, DB, OTSG\}$<br>$HRSG$ - Heat Recovery Steam Generator<br>$DB$ - Drum Boiler<br>$OTSG$ - Once Through Steam Generator |
| $tu \in TU$ | Treatment units<br>$tu \in \{ST, IGF, ORF, HCY, LS, EVAP, WAC\}$<br>$ST$ - Skim Tank<br>$IGF$ - Induced Gas Flotation<br>$ORF$ - Oil Removal Filter<br>$HCY$ - Hydrocyclone<br>$LS$ - Lime Softener<br>$EVAP$ - Evaporator<br>$WAC$ - Weak Acid Cation Exchanger |
| $WI$ | Well Injection |

**Flow variables (in tonne/hr)**

| | |
|---|---|
| $F^{final}$ | Outflow from final discharge mixer in the small water treatment model |
| $F_{s,tu}$ | Flow from source $s$ splitter to $tu$ pre-mixer |

| | |
|---|---|
| $F_{sgu}^{bbd,rec}$ | Recycle flow from $sgu$ to $s \in \{BBD\}$ as boiler blowdown in the SAGD model |
| $F_{sgu}^{in}$ | Inflow to $sgu$ in the SAGD model |
| $F_{sgu}^{out}$ | Outflow from $sgu$ in the SAGD model |
| $F_s$ | Flow rate of source water from $s$ in the small water treatment model |
| $F_{tu,sgu}^{exit}$ | Flow from $tu$ post-splitter to $sgu$ pre-mixer in the SAGD model |
| $F_{tu,tu'}^{rec}$ | Recycle flow from $tu$ to $tu'$ |
| $F_{tu}^{exit}$ | Flow from $tu$ post-splitter to final discharge mixer in the small water treatment model |
| $F_{tu}^{in}$ | Inflow to $tu$ |
| $F_{tu}^{out}$ | Outflow from $tu$ |
| $F_{WI}^{in}$ | Inflow to $WI$ in the SAGD model |

**Concentration variables (in ppm)**

| | |
|---|---|
| $C_c^{final}$ | Concentration of $c$ in final discharge stream in the small water treatment model |
| $C_{sgu,c}^{in}$ | Concentration of $c$ in inlet to $sgu$ in the SAGD model |
| $C_{tu,c}^{in}$ | Concentration of $c$ in inlet to $tu$ |
| $C_{tu,c}^{out}$ | Concentration of $c$ in outlet from $tu$ |

# Chapter 1

# Introduction

## 1.1 Motivation

The development of large-scale wastewater treatment procedures has been gaining increasing attention since the era of industrialization. In the past, effluent treatment mainly focussed on sewage treatment, and filtration techniques for water purification to standards appropriate for human consumption and use. However, the advent of industrialization also brought about various new technologies for the treatment of effluents containing a more diverse profile of pollutants. In the early 1900s, new technologies such as the activated sludge process emerged, leading to a period of increased understanding of wastewater and its treatment. Simultaneously, modern industrialization also brought about a need for regulation of, and standards imposed on disposed effluent streams, to stay within environmental guidelines and norms. Thus, this increased understanding and motivation to improve wastewater treatment technology lead to the development of a number of procedures such as membrane filtration, nanofiltration, and reverse osmosis, as well as bioreactors, and improved physical treatment processes [3].

## 1.2 Introduction to effluent treatment

Present day effluent treatment is classified into a series of stages - primary, secondary, and tertiary stages. Primary treatment comprises physical procedures to remove contaminants such as oil and suspended solids, while secondary treatment consists of biological and chemical treatments. Tertiary treatment techniques are generally used for the treatment of residual contaminants [4]. Effluent is passed through a network of treatments classified under these stages. A summary of the overall requirements for an effluent treatment system is given as follows [3].

- Optimal sequencing of treatment procedures
- Optimal distribution of flow rate, and thus, mass load of pollutants through the treatments
- Flexibility to handle varying source flow rates and variation in pollutant loads

In the past, effluent treatment was conducted through a centralized approach. In centralized treatment, all effluent streams are mixed and treated in a common facility, where the mixed stream is passed through all chosen treatment units. In contrast, in the decentralized approach, different effluent streams are treated separately or fractionally mixed. The decentralized approach offers more advantages than the centralized approach since the former reduces the amount of flow to be processed as compared to the latter ([5], [6]), and most treatment unit operational costs increase as a function of inflow [7]. Therefore, the need for a systematic design of an effluent treatment network has been well-recognized and tackled by various authors in the literature.

## 1.3 The "pooling" problem

The design of effluent treatment networks is a subset of the "pooling problem". The general pooling problem seeks the optimal solution to transporting entities across a flow network from source nodes to destination nodes, at minimum cost, while meeting imposed limitations and targets. It can be stated as follows - what is the optimal solution to mixing materials from various source nodes, within a network of intermediate nodes (termed as pools), to satisfy the targets at the demand nodes [8]? Such problems arise in a variety of applications; chief among these is the petrochemical industry, wastewater treatment facilities, and chemical plants. A schematic of the pooling problem is shown in Figure 1.1 [8].

The flow variables between the nodes, and the concentration variables at each node in the pooling problem are decision variables to be optimized by the model. Hence, the pooling problem contains bilinear terms, and is a special case of the non-convex quadratic program with quadratic constraints (QCQP). The pooling problem has been recognized to be NP-hard [9]. This problem has been solved for optimal solutions using a variety of techniques. The pooling problem contains features from two well-studied classes of problems in optimization - the network flow problem, and the blending problem. When intermediate pools are unnecessary, the pooling problem

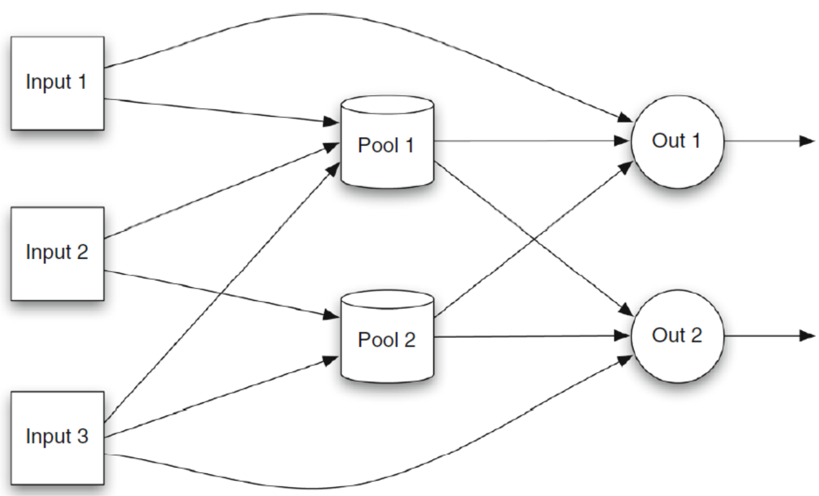


Figure 1.1: Schematic representation of the pooling problem

tends to a general blending problem. It can, thus, be formulated as a mixed-integer nonlinear programming problem (MINLP), in which the binary variables account for the existence of flow streams between various nodes. The pooling problem has mainly been formulated in two ways - the $p$ formulation, and the $q$ formulation [10]. The $p$ formulation of the pooling problem utilizes flow and quality variables, whereas the $q$ formulation replaces the quality variables with flow proportions. It has been documented that the $q$ formulation performs better when utilized with branch-and-bound algorithms, than the $p$ formulation. Sahinidis and Tawarmalani (2005) [11] added nonlinear constraints to this model to strengthen the lower bounding step in the generic branch-and-bound algorithm, without adding further complexity to the search process, and termed this formulation the $pq$ formulation, It was proven that the $pq$ approach reduced the size of the branch-and-bound tree.

The pooling problem has been solved using a variety of local and global optimization techniques. Haverly (1978) [12] solved the pooling problem using a linear programming (LP) approach, in which all the quality variables were fixed to their anticipated value and the resulting LP model was solved for flow variables. The quality of the solution was, therefore, found to be heavily dependent on the initial guess provided. The problem was also solved using successive linear programming (SLP), in which the bilinear terms are replaced by their first order Taylor series expansion [13]. The first global optimization approach for the pooling problem was developed by Floudast and Visweswaran (1990) [14]. In this approach, the original non-convex nonlinear problem is decomposed into primal and relaxed dual subproblems. The approach utilizes the concepts of duality, and Lagrangian decomposition to obtain the global optimum. Since this approach, most of the work towards global optimization of the pooling problem has been focused on applying different relaxation techniques to the global optimization framework, such as the piecewise linear relaxation technique adopted by Gounaris, et al. (2009) [15].

## 1.4 Survey of methods for optimal design of deterministic water networks

The design of effluent treatment networks, in particular, has been studied in literature using a number of techniques. A well-studied approach to this problem is the use of pinch analysis. Pinch analysis is an engineering design technique that minimises the energy consumption of a process using thermodynamic relations and constraints. El-Halwagi and Manousiouthakis (1989) [16] have synthesised mass exchange networks for single pollutants using pinch analysis, and extended the technique to multicomponent networks. Wang and Smith (1994) [17] have developed the design of a wastewater treatment network using graphical representations and techniques for streams with a single pollutant, and treated the multi-component contaminant case as an extension to the single-component case. Kuo and Smith (1997) [18] improved the multi-component wastewater treatment network design problem statement developed by Wang, et al. [17]. Other authors have also approached the problem of optimal design of wastewater networks in the context of mathematical optimization. Hamad, et al. (1996) [19] synthesized waste-interception networks to tackle gaseous as well as liquid phase pollution in an integrated framework, by removal of contaminants from intermediate plant streams, rather than terminal streams. They formulated the problem as a mixed-integer nonlinear program (MINLP), and used graphical representations to track the pollutant level through the process to determine the interception policies. Alva-Argaez, et al. (1998) [20] combined the inferences from pinch analysis of combinatorial water networks, along with a recursive decomposed MILP approach to optimize the superstructure. Savelski and Bagajewicz (2001) [21] proposed a linear programming (LP) approach to optimally solving the design of effluent treatment networks for a single contaminant based on previously developed necessary conditions of optimality. They also proposed solving a series of mixed-integer linear programs (MILP) to solve for different network alternatives. Jezowski, et al. (2006) [22] proposed a sequential approach to the design of industrial effluent treatment networks by developing an initial structure using pinch analysis and effluent degradation insights, and further improving this structure through mathematical optimization. Castro, et al. (2006) [23] developed a heuristic method for the optimal design of wastewater treatment networks by generating multiple solutions using a new linear formulation of the original model to be used as initial solutions for the optimization of the original nonlinear model. Misener and Floudas (2010) [24] considered the wastewater network optimization as a pooling problem, and solved it using quadratically constrained MINLP models to reduce the number of bilinear terms in the model, in addition to introducing methods to tighten the relaxation. Galan and Grossmann (1998) [1] solved the design of the nonlinear effluent treatment system model, introduced by Wang and Smith [17] using a heuristic global optimization algorithm. They used linear models obtained through the substitution of bilinear terms with McCormick envelopes. They also proposed a solution strategy when the design problem involves the selection of treatment units, in addition to optimization of the design network. In this thesis, the superstructure used by Galan and Grossmann [1] is used as the reference water treatment model. Furthermore, the use of the relaxed LP formulation using McCormick envelopes is explored in Chapter 2 of the thesis. In another publication [25], they evaluated a heuristic search procedure for the global optimum through the successive relaxation of a relaxed linear formulation, and the original nonlinear model, using numerous objective functions in the relaxed formulation, for the design of a multicomponent case.

In addition to effluent treatment for safe disposal, the optimal design of effluent treatment networks in the context of steam-assisted gravity drainage (SAGD) reservoirs has been studied by Forshomi, et al. (2017) [2]. The SAGD reservoir has proven to be an energy intensive process, with high water consumption [26]. In this work, the authors discuss and explore the economic and environmental trade-offs that result from generation of steam using treated effluent within a SAGD reservoir. The solution strategy employed in this work uses the approach detailed by Alva-Argaez, et al. [20]. This model is used as a large-scale case study in Chapter 5 of this thesis.

## 1.5 Survey of methods for optimal design of water networks under uncertainty

The techniques discussed above for the optimal design of effluent treatment networks assumes that the problem is deterministic in nature, that is, all parameters in the model are exactly known and are unaffected by perturbation of any kind. However, studies strongly suggest that the operation of the effluent treatment network is affected significantly by perturbations in various parameters such as source flow rate, inlet concentrations, and treatment unit performance efficiency [27]. Figure 1.2 [28] shows the variation in the removal efficiency of a reverse osmosis plant with respect to six contaminants, over the course of one month. As evidenced from the plot, considerable perturbations exist in the operation of an effluent treatment system, and so, the deterministic optimal design of such networks is impractical.

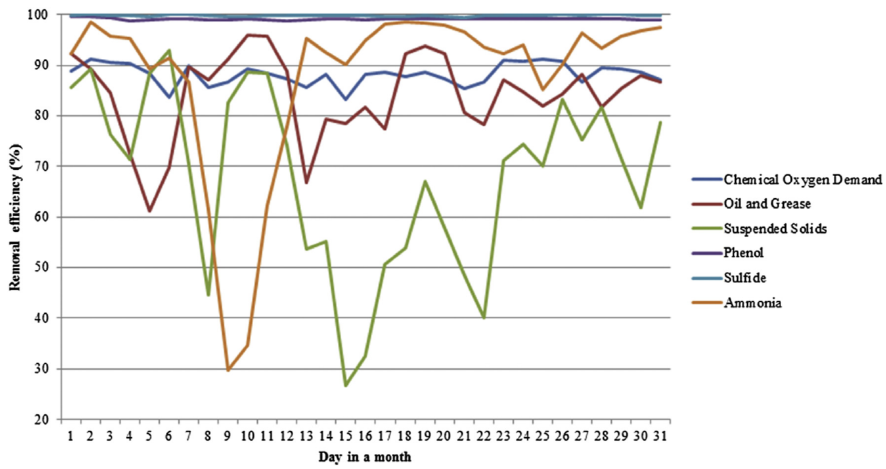


Figure 1.2: Variation in the contaminant removal efficiency of a reverse osmosis unit over a one-month period

Therefore, the synthesis of effluent treatment, or more generally, water networks under uncertainty is a more practically applicable problem statement. Certain works in literature have attempted to solve the water network optimization problem under uncertainty. Halemane and Grossmann (1983) [29] proposed a rigorous mathematical formulation for optimal process design under uncertainty. Antunes, et al. (2012) [30] evaluated a robust optimization approach to the planning of regional wastewater systems under discharge destination flow uncertainty, using and enhanced simulated annealing algorithm. Koppol and Bagajewicz (2003) [31] addressed the optimal design of effluent treatment network synthesis under contaminant load uncertainty. In this work, they assumed that the contaminant mass load followed a bounded uniform distribution, and solved the model for a set of discrete realizations of uncertainty. The work also addresses the concept of financial risk management on the network cost. Al-Redhwan, et al. (2005) [32] used a two-stage stochastic programming formulation of the fixed-load water network model to solve for optimal design of the network under mass load uncertainty. Karuppaiah and Grossmann (2008) [33] solved the problem in a two-stage approach using McCormick's envelopes for relaxation of the bilinear terms, using a Lagrangian decomposition technique on the multiscenario model. Kang and

Lansey (2013) [34] addressed the optimal design of wastewater infrastructure using scenario-based robust optimization under uncertain water demand.

## 1.6 Optimization under uncertainty

The field of optimization under uncertainty was initiated by Dantzig [35]. This field of optimization is called stochastic programming, where the underlying probability distribution of uncertain parameters or variables is assumed to be known or can be estimated. Another approach to optimization under uncertainty is called robust optimization, initially put forward by Soyster [36]. The aim of robust optimization is to find a solution that is optimal against the worst-case realization of uncertainty for that set. In the following sections, a brief description of stochastic and robust optimization techniques is detailed. Sahinidis (2004) [37] published a review of the significant techniques developed, and in use, for optimization under uncertainty.

### 1.6.1 Adaptive/recourse stochastic programming

One method to deal with stochastic programs is the two-stage or recourse approach. In this method, the decisions in the model are classified into two types - here-and-now/first stage decisions, and wait-and-see/second stage decisions. The first stage decisions occur before the realization of uncertainty, while the second stage decisions occur after the uncertainty has been realized. The general form of the two-stage recourse stochastic programming problem is given as follows, using the formulation from Birge and Louveaux (1997) [38].

$$\begin{aligned}
&\min_{x,y(\xi)} \quad c^\top x + E[q(\xi)^\top y(\xi)] \\
&\text{subject to} \\
&Ax \geq b \\
&T(\xi)x + Wy(\xi) \geq h(\xi) \\
&x \geq 0, \quad y(\xi) \geq 0
\end{aligned}$$

The objective of this optimization problem is to minimize the cost of the first stage decisions (independent of uncertainty), plus the expected cost of the second stage decisions (dependent on uncertainty). The first set of constraints contains only first stage decision variables, while the second set of constraints is dependent on uncertainty. This program is solved for a finite number of scenarios, denoted by $K$. This approach is also called scenario-based recourse programming. In this method, a finite set ($K$) of realizations of uncertainty, termed as 'scenarios', are generated [39]. The optimization problem is then tasked with finding a solution that is optimal against each scenario. The number of scenarios generated affects the computational effort required to solve the model. Scenarios are normally generated by discretization, and a positive weight ($p_k$) is assigned to each scenario ($k \in K$). This weight $p_k$ depicts the probability of occurrence of scenario $k$. However, as the dimension of the primitive uncertainty vector increases, the total number of scenarios to be generated increases exponentially, making the discretization approach unsuitable for scenario generation [40]. In such cases, methods such as Monte Carlo sampling have proven useful for scenario generation. In the most general case of recourse programming, scenarios are obtained for each stage of the program, and can be depicted in the form of a "scenario tree", or "scenario fan" (Figure 1.3). The general recourse program formulation for a two-stage program is given as follows.

$$\begin{aligned}
&\min_{x,y_k} \quad c^\top x + \sum_{k=1}^{K} p_k q_k^\top y_k \\
&\text{subject to} \\
&Ax \geq b \\
&T_k x + W y_k \geq h_k, \quad k = 1, ..., K \\
&x \geq 0, \quad y_k \geq 0, \quad k = 1, ...K
\end{aligned}$$

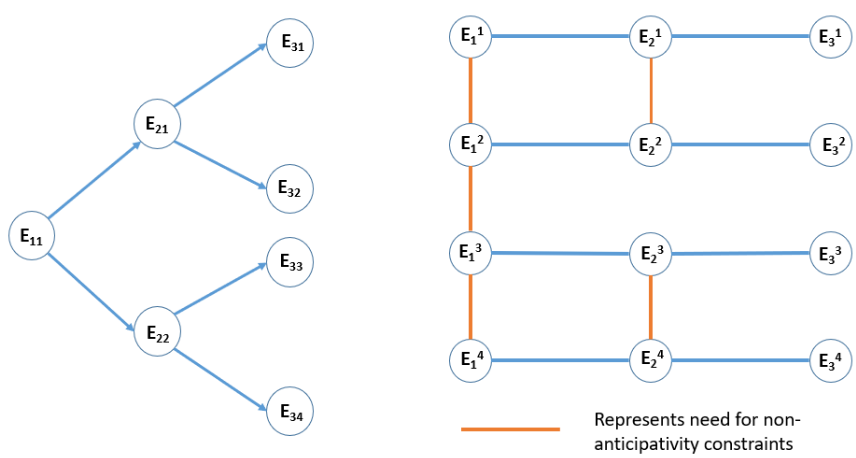


Figure 1.3: Schematic representation of scenario formulation for multistage recourse programming using the scenario tree (left) and scenario fan (right) formulations

As the number of scenarios ($K$) increases, the size of the model increases, and it becomes computationally intensive. Some approaches such as stochastic decomposition, Benders' decomposition, etc. have been proposed to deal with such large-scale stochastic problems. Acevedo and Pistikopoulos (1998) [41] presented a framework to handle process synthesis under uncertainty using stochastic optimization.

### 1.6.2 Chance constrained programming

Stochastic programming problems can also be solved as chance constrained programs. In this method, constraints are implemented with a specified confidence limit [42]. The magnitude of the confidence limit is inversely proportional to the probability of violation of the constraint. The general formulation of the chance constrained model is given below.

$$\begin{aligned}
&\min_{x} \quad c^\top x \\
&\text{subject to} \\
&P\big(A^\top(\xi)x \geq b(\xi)\big) \geq 1-\alpha \\
&x \in X
\end{aligned}$$

In the above model, the probability that all constraints contained in the model are jointly feasible must be above $(1-\alpha)$, where $\alpha \in [0,1]$. This type of problem is called the joint chance constrained problem. A variation to this model can be made, where the probability of violation of each constraint is individually provided with specific values of $\alpha$. Such problems are called individual chance constrained problems.

### 1.6.3 Static robust optimization

In situations where the probability distribution of the uncertain/random parameters is known, stochastic programming techniques prove to be useful tools for optimization under uncertainty. However, when the distribution information is unavailable, a more conservative solution is desired, in order to obtain a solution that is feasible for all realizations of uncertainty. Uncertainty in the optimization model is addressed by solving the model for the worst case of uncertainty realizable, and this is termed as static robust optimization. In this method, all decisions are to be made before the realization of uncertainty. The general form of a linear optimization problem under uncertainty is given as follows.

$$
\begin{aligned}
&\min_{x} \quad c^\top x\\
&\text{subject to}\\
&Ax \geq b\\
&\{c, A, b\} \in U
\end{aligned}
$$

In the above model, it is assumed that the cost coefficients, $A$, and $b$ are affected by uncertainty. The robust counterpart of this model is given as follows.

$$
\begin{aligned}
&\min_{x} \quad \max_{c \in U} \quad c^\top x\\
&\text{subject to}\\
&\underset{\{a_i, b_i \in U_i\}}{max} a_i^\top x \leq b_i, \quad \forall i
\end{aligned}
$$

Using the static robust optimization technique, a conservative solution is found by satisfying the constraints for the worst-case realization of uncertainty in the uncertainty set defined, such that the solution may be feasible for all other realizations of uncertainty.

### 1.6.4 Decision rule-based optimization

In contrast to static robust optimization, in dynamic robust optimization, first stage decisions are made without any knowledge of the realized uncertainty, while second stage decisions are made after uncertainty has been realized. This adjustable optimization approach has been applied to practical cases such as scheduling of industrial chemical processes ([43], [44]). Ben-Tal, et al. [45] proposed an affinely adjustable decision rule formulation for the recourse decisions in the robust model. In this approach, the second stage decision is assumed to be a linear function of uncertainty.

Given the general two-stage optimization problem under uncertainty,

$$
\begin{aligned}
&\min_{x,y(\xi)} \quad c^\top x \\
&\text{subject to} \\
&Ax \geq b \\
&T(\xi)x + Wy(\xi) \geq h(\xi), \quad \forall \xi \in \Xi
\end{aligned}
$$

the affine adjustable robust counterpart (AARC) is given as,

$$
\begin{aligned}
&\min_{x,y^0,y^1} \quad c^\top x \\
&\text{subject to} \\
&Ax \geq b \\
&T(\xi)x + W(y^0 + y^1\xi) \geq h(\xi), \quad \forall \xi \in \Xi
\end{aligned}
$$

The AARC approach uses the linear decision rule to provide the user with the capacity to make second stage decisions after uncertainty has been realized, in the form of a linear policy, although no guarantee exists that the optimal solution follows a linear policy. The procedure to obtain the adjustable affine robust counterpart to a constraint in an optimization model under uncertainty has been detailed by Ben-Tal, et al. [45]. This procedure is detailed below.

Let a general recourse decision $z(\xi)$ be an affine function of uncertainty $\xi$, as follows.

$$z(\xi) = z^0 + z^1\xi \tag{1.1}$$

Substituting the affine formulation of $z(\xi)$, presented in Equation 1.1, into the constraints of the model yields a set of semi-infinite constraints, for every possible realization of $\xi$, making the model intractable. In order to construct the finite, tractable counterpart, the property of duality of linear programming problems is used. Ben-Tal, et al. (2004) [45] developed the methodology to obtain the tractable, robust counterpart to the uncertain inequality constraints resulting from reformulation of the variables using the affine decision rule.

Consider the stochastic programming problem:

$$
\begin{aligned}
&\min_{x_1,x_2,z(\xi)} \quad c_{x_1}x_1 + c_{x_2}x_2 + E[c_z z(\xi)] \\
&\text{subject to} \\
&x_1 + z(\xi) \geq D(\xi), \quad \forall \xi \in \Xi \\
&x_2 + z(\xi) = a_1, \quad \forall \xi \in \Xi \\
&x_1, x_2 \geq 0 \\
&z(\xi) \geq 0, \quad \forall \xi \in \Xi
\end{aligned}
$$

Applying the ADR to the problem using the following relations,

$$
\begin{aligned}
&D(\xi) = \xi D^1 + (1-\xi)D^2 \\
&z(\xi) = z^0 + z^1\xi
\end{aligned}
$$

gives the semi-infinite intractable model,

$$
\begin{aligned}
&\min_{x_1,x_2,z^0,z^1} \quad c_{x_1}x_1 + c_{x_2}x_2 + c_z(z^0 + z^1 E[\xi]) \\
&\text{subject to} \\
&x_1 + z^0 + z^1\xi \geq \xi D^1 + (1-\xi)D^2, \quad \forall \xi \in \Xi \\
&x_2 + z^0 + z^1\xi = a_1, \quad \forall \xi \in \Xi \\
&x_1, x_2 \geq 0 \\
&z^0 + z^1\xi \geq 0, \quad \forall \xi \in \Xi
\end{aligned}
$$

where $D^1$ and $D^2$ are the extreme points for the realization of $\xi$. The finite tractable counterpart for each inequality constraint is obtained through the property of duality of linear programming. The process of obtaining the finite tractable counterpart is illustrated below for the first inequality constraint.

$$
x_1 + z^0 + z^1\xi \geq \xi D^1 + (1-\xi)D^2, \quad \forall \xi \in \Xi
$$

$$
\downarrow
$$

$$x_1 + z^0 + z^1\xi \geq \xi D^1 + D^2 - \xi D^2, \quad \forall \xi \in \Xi$$

$$\downarrow$$

$$(x_1 + z^0 - D^2) + \xi(z^1 - D^1 + D^2) \geq 0, \quad \forall \xi \in \Xi$$

The primitive uncertainty $\xi$ is considered, in the simplest case, to be a scalar value with specified lower and upper limits, $\xi^{low}$ and $\xi^{high}$, respectively, as follows.

$$\xi^{low} \leq \xi \leq \xi^{high}$$

The uncertainty set $\Xi$ is specified in the form $\mathbf{A}\xi \geq \mathbf{b}$, as follows.

$$\begin{bmatrix} 1 \\ -1 \end{bmatrix} \xi \geq \begin{bmatrix} \xi^{low} \\ -\xi^{high} \end{bmatrix}$$

It is to be noted that the same structure can be adopted even if the primitive uncertainty $\xi$ is a vector. In that case too, $\mathbf{A}$ and $\mathbf{b}$ are used to contain the lower and upper limit specifications on each member of the vector $\xi$. When $\xi$ is a vector, the slope term $z^1$ in the LDR formulation of the recourse variable, is a column vector of the same dimensions as that of $\xi$.

Using the matrix formulation for $\Xi$ specified above, the constraint (in the form of the $\geq$ inequality) is rewritten using the *min* operator, as follows,

$$(x_1 + z^0 - D^2) + \begin{bmatrix} \min\limits_{\xi} \quad \xi(z^1 - D^1 + D^2) \\ \text{subject to} \\ \boldsymbol{A}\xi \geq \boldsymbol{b} \end{bmatrix} \geq 0$$

The dual of the inner minimization problem is obtained as a *max* problem, as follows,

$$(x_1 + z^0 - D^2) + \begin{bmatrix} \max\limits_{\boldsymbol{\lambda} \geq 0} \quad (b^\top \boldsymbol{\lambda}) \\ \text{subject to} \\ \boldsymbol{A}^\top \boldsymbol{\lambda} = z^1 - D^1 + D^2 \end{bmatrix} \geq 0$$

where, the dimensions of $\lambda$ are the same as those of $\mathbf{b}$. The *max* operator is dropped and the following counterpart is obtained.

$$
\begin{aligned}
&(x_1 + z^0 - D^2) + b^\top \boldsymbol{\lambda} \geq 0 \\
&\boldsymbol{A}^\top \boldsymbol{\lambda} = z^1 - D^1 + D^2 \\
&\boldsymbol{\lambda} \geq 0
\end{aligned}
$$

The final adjustable affine robust counterparts to all the inequality constraints in the model are formulated using the approach detailed above. It is to be noted that in the case of equality constraints involving $\xi$, the coefficients of $\xi$ are equated to 0 to obtain the robust counterpart. Therefore, the final robust counterpart for the stochastic programming model is given as follows.

$$
\begin{aligned}
&\min_{x_1, x_2, z^0, z^1} \quad c_{x_1} x_1 + c_{x_2} x_2 + c_z (z^0 + z^1 E[\xi]) \\
&\text{subject to} \\
&(x_1 + z^0 - D^2) + b^\top \boldsymbol{\lambda} \geq 0 \\
&\boldsymbol{A}^\top \boldsymbol{\lambda} = z^1 - D^1 + D^2 \\
&x_2 + z^0 - a_1 = 0 \\
&z^1 = 0 \\
&x_1, x_2 \geq 0 \\
&z^0 + b^\top \lambda_z \geq 0 \\
&A^\top \lambda_z = z^1 \\
&\boldsymbol{\lambda} \geq 0
\end{aligned}
$$

## 1.7 Thesis structure

In this thesis, the linear decision rule (LDR) approach was applied in three different ways. In Chapter 2, the water treatment model was first relaxed, using McCormick envelopes, into the form of an LP, and the linear decision rule formulation was applied to the recourse variables in the model. In Chapter 3, the model was linearized around its nominal conditions using first order Taylor series approximation, and then, the LDR formulation was applied to the recourse variables. In Chapter 4, the novel nonlinear robust optimization approach developed by Yuan, et al. (2018) [46], was applied to the model. The same approach was applied to a large-scale case study, the SAGD effluent treatment and steam generation network, in Chapter 5. A summary is provided in Chapter 6, along with possible future work along similar lines to the work in the thesis. The methods applied in this thesis were mainly formulated keeping in mind industrial process wastewater treatment, with uncertain flow rates, and can possibly be extended to dealing with uncertainty in treatment efficiencies as well as contaminant concentrations.

# Chapter 2

# Linear Stochastic Optimization using McCormick Envelopes

In this chapter, the application of the McCormick relaxation technique to the small water treatment NLP (nonlinear programming) model is discussed. The model description was obtained from a work by Grossmann, et al. [1] detailing a successive solution procedure using McCormick relaxation of nonlinear deterministic models to obtain global/near global optimum solutions on non-convex, nonlinear models. The concept of relaxation of nonlinear models using McCormick envelopes is explained in Section 2.1. Section 2.2 provides background on the small water treatment model chosen as a case study in this thesis, and Section 2.3 presents its deterministic formulation and discusses its solution. The relaxed LP formulation of the model is presented in Section 2.4. The derivation and solution of the stochastic LDR-based formulation of the relaxed LP model is presented and analyzed in Section 2.5. Section 2.6 presents concluding remarks.

## 2.1 Relaxation using McCormick Envelopes

Commonly-used NLP (nonlinear programming) solvers in GAMS, such as IPOPT and CONOPT, do not guarantee a global optimum solution for non-convex models. To address this shortcoming, Galan and Grossmann (1998) [1] suggested a four-step approach to obtain a good upper bound on the global optimum of the NLP model. This approach involves the successive solution of the relaxed LP formulation, with the original non-convex nonlinear model. In this thesis, the relaxed LP model was formulated from the NLP model using McCormick envelopes for the bilinear terms in the model equations. The solution to this relaxed LP problem provided a lower bound on the optimal solution of the original NLP. Using McCormick envelopes, each bilinear term in the model equation was substituted with a single new variable; this new variable was then constrained using the upper and lower bounds on the original variables in the bilinear term.

The use of duality to obtain the robust counterpart of inequality constraints is well defined [45] only for constraints linear in uncertainty. Consider a general bilinear term denoted by $x \cdot y$. Accounting for the dependence of $x$ and $y$ on uncertainty ($\xi$), the bilinear term is denoted by $x(\xi) \cdot y(\xi)$. When the variables are redefined using the LDR formulation, constraints containing these bilinear terms become nonlinear in uncertainty; specifically, in this case, they become quadratic in uncertainty. This is illustrated below.

$$\begin{aligned} x(\xi) \cdot y(\xi) &= (x^0 + x^1\xi)(y^0 + y^1\xi) \\ &= x^0y^0 + \xi(x^1y^0 + x^0y^1) + \xi^2(x^1y^1) \end{aligned}$$

Hence, there is a need to make a linear approximation of the constraints containing bilinear terms, in order to apply the affine decision rule to solve a stochastic linear optimization problem using LDR. This linear approximation can be performed by relaxing the NLP model using McCormick envelopes to obtain the LP formulation. Consider a general optimization problem as follows.

$$\begin{aligned} &\min_{x,y} \quad \phi(x,y) \\ &\text{subject to} \\ &F(x,y) = 0 \\ &G(x,y) \geq 0 \\ &\underline{x} \leq x \leq \overline{x}, \quad \underline{y} \leq y \leq \overline{y} \end{aligned}$$

Substituting the bilinear terms $xy$ in $F(x,y)$ and $G(x,y)$ with $w$, the relaxed model is given as follows.

$$
\begin{aligned}
&\min_{x,y,w} \quad \phi(x,y,w) \\
&\text{subject to} \\
&F(x,y,w) = 0 \\
&G(x,y,w) \geq 0 \\
&w \geq \underline{x}y + x\underline{y} - \underline{x}\underline{y} \\
&w \geq \overline{x}y + x\overline{y} - \overline{x}\overline{y} \\
&w \leq \underline{x}y + x\overline{y} - \underline{x}\overline{y} \\
&w \leq \overline{x}y + x\underline{y} - \overline{x}\underline{y} \\
&\underline{x} \leq x \leq \overline{x}, \quad \underline{y} \leq y \leq \overline{y}
\end{aligned}
$$

**Illustrative example** The derivation of the relaxed LP formulation of a model containing bilinear terms is illustrated in the following example. The original NLP model is given as follows.

$$
\begin{aligned}
&\min_{x,y} \quad - xy - 2x \\
&\text{subject to} \\
&xy \leq 12 \\
&0 \leq x \leq 6, \quad 0 \leq y \leq 3
\end{aligned}
$$

The relaxed LP formulation is given as follows.

$$
\begin{aligned}
&\min_{x,y,w} \quad - w - 2x \\
&\text{subject to} \\
&w \leq 12 \\
&w \geq 0 \\
&w \geq 6y + 3x - 18 \\
&w \leq 3x \\
&w \leq 6y \\
&0 \leq x \leq 6, \quad 0 \leq y \leq 3
\end{aligned}
$$

## 2.2 Overview of the small water treatment model

The small water treatment model used as a case study in this report considers two process flow streams ($s_1$ and $s_2$) containing two contaminants ($A$ and $B$), a set of two treatment units ($tu_1$ and $tu_2$) and a final discharge stream. Each process stream is equipped with a splitter and each treatment unit is equipped with a pre-mixer and a post-splitter. The final discharge from each treatment unit is mixed, and disposed. Target concentrations for each contaminant in the process streams is specified for the final discharge stream. The objective of this optimization exercise was to minimize the total flow through the treatment units. The superstructure and the general network are shown in Figure 2.1.

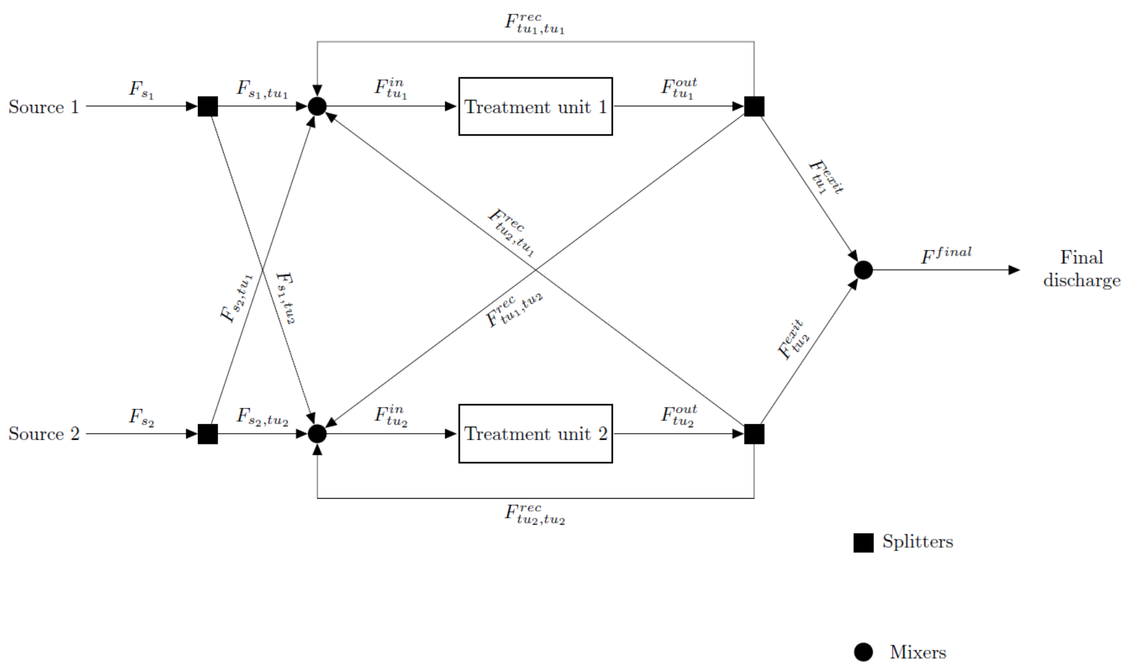


Figure 2.1: Schematic representation of the small water treatment model

## 2.3 Deterministic formulation

The small water treatment model is described by a set of mass flow, and component concentration balances over all the units in the model. The objective function is given by Equation 2.3. Equations 2.2 - 2.6, and 2.7 - 2.10 describe the flow balances and component balances respectively, and the concentration limits on the final stream are

Table 2.1: Decision variables in the small water treatment model

| Variable | Description |
|---|---|
| | Flow variables (tonne/hr) |
| $F_{s,tu}$ | Exit flow from splitter to treatment unit |
| $F_{tu}^{in}$ | Inflow to treatment unit |
| $F_{tu}^{out}$ | Outflow from treatment unit |
| $F_{tu,tu'}^{rec}$ | Recycle flow between treatment units |
| $F_{tu}^{exit}$ | Exit flow from treatment unit to final mixer |
| $F^{final}$ | Outflow from final mixer |
| | Concentration variables (ppm) |
| $C_{tu,c}^{in}$ | Concentration of contaminant in inflow to treatment unit |
| $C_{tu,c}^{out}$ | Concentration of contaminant in outflow from treatment unit |
| $C_{c}^{final}$ | Concentration of contaminant in outflow from final mixer |

Table 2.2: Auxiliary parameters in the small water treatment model [1]

| | Parameters (units) | | |
|---|---|---|---|
| $F_s$ | Source flow rate under nominal conditions (tonne/hr) | | 40 |
| $C_{s,c}$ | Source flow contaminant concentration (ppm) | $s_1, A$ | 100 |
| | | $s_1, B$ | 20 |
| | | $s_2, A$ | 15 |
| | | $s_2, B$ | 200 |
| $RR_{tu,c}$ | Treatment unit efficiency | $tu_1, A$ | 0.95 |
| | | $tu_1, B$ | 0 |
| | | $tu_2, A$ | 0 |
| | | $tu_2, B$ | 0.976 |
| $C_c^{target}$ | Target concentration for the final stream (ppm) | $A$ | 10 |
| | | $B$ | 10 |

described by Equation 2.11. The sets of variables optimized in this model are listed in Table 2.1, and the parameters used are listed in Table 2.2 [1].

$$\min \quad \sum_{tu} F_{tu}^{in} \tag{2.1}$$

subject to

$$F_s = \sum_{tu} F_{s,tu}, \quad \forall s \in S \tag{2.2}$$

$$\sum_{s} F_{s,tu} + \sum_{tu'} F^{rec}_{tu',tu} = F^{in}_{tu}, \quad \forall tu \in TU \tag{2.3}$$

$$F^{in}_{tu} = F^{out}_{tu}, \quad \forall tu \in TU \tag{2.4}$$

$$F^{out}_{tu} = \sum_{tu'} F^{rec}_{tu,tu'} + F^{exit}_{tu}, \quad \forall tu \in TU \tag{2.5}$$

$$\sum_{tu} F^{exit}_{tu} = F^{final} \tag{2.6}$$

$$\sum_{s} F_{s,tu} C_{s,c} + \sum_{tu'} F^{rec}_{tu',tu} C^{out}_{tu',c} = C^{in}_{tu,c} F^{in}_{tu}, \quad \forall tu \in TU, c \in C \tag{2.7}$$

$$C^{in}_{tu,c} F^{in}_{tu} = C^{out}_{tu,c} F^{out}_{tu} + C^{in}_{tu,c} F^{in}_{tu} RR_{tu,c}, \quad \forall tu \in TU, c \in C \tag{2.8}$$

$$F^{out}_{tu} C^{out}_{tu,c} = \sum_{tu'} F^{rec}_{tu',tu} C^{out}_{tu,c} + F^{exit}_{tu} C^{out}_{tu,c}, \quad \forall tu \in TU, c \in C \tag{2.9}$$

$$\sum_{tu} F^{\text{exit}}_{tu} C^{\text{out}}_{tu,c} = C^{\text{final}}_{c} F^{\text{final}}, \quad \forall c \in C \tag{2.10}$$

$$C^{\text{final}}_{c} \leq C^{\text{target}}_{c}, \quad \forall c \in C \tag{2.11}$$

The deterministic model was solved at nominal conditions ($F_s = 40$ tonne/hr $\forall s \in S$) on GAMS using the ANTIGONE NLP solver. The locally optimal objective magnitude was found to be 89.8361 tonne/hr, and the resulting optimal network is depicted in Figure 2.2. It was observed that $s_1$ was diverted entirely through $tu_1$, and $s_2$ entirely through $tu_2$. A recycle stream from $tu_1$ to $tu_2$ was also observed. The target concentrations in the final stream were exactly met.

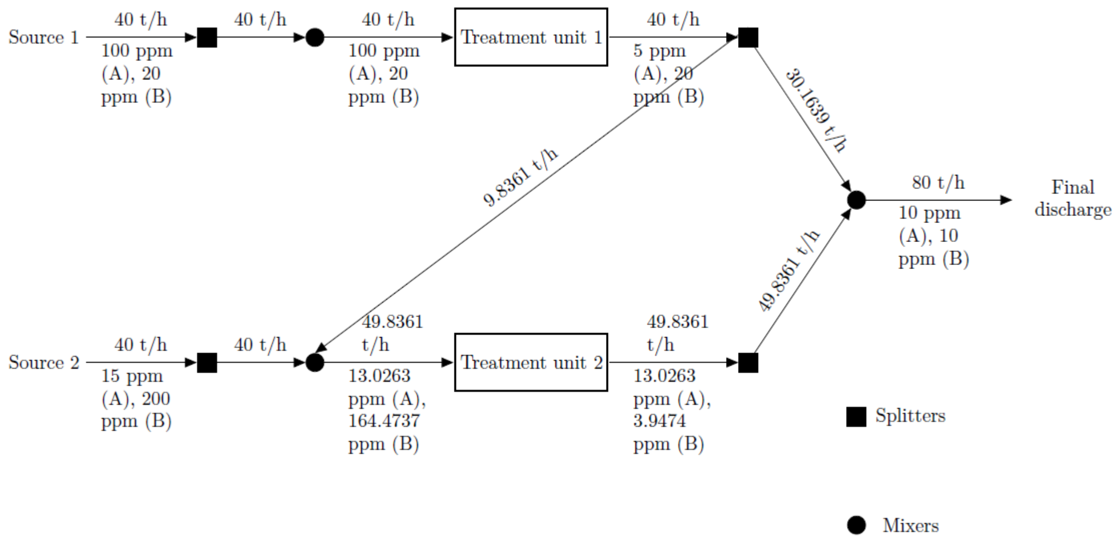


Figure 2.2: Optimal solution for the deterministic formulation of the small water treatment model

## 2.4 Relaxed LP formulation

Using the McCormick relaxation technique detailed in Section 2.1, the relaxed LP formulation of the small water treatment model was derived. The bilinear terms in Equations 2.7 - 2.10 were replaced by the variables $W^{rec}_{tu',tu,c}$, $W^{in}_{tu,c}$, $W^{out}_{tu,c}$, $W^{exit}_{tu,c}$ and $W^{final}_{c}$. The lower and upper limits on the flow and concentration terms involved in the bilinear terms were computed using the total source flow, and maximum source contaminant concentration values, as depicted in Table 2.3.

$$\min \quad \sum_{tu} F^{in}_{tu} \tag{2.12}$$

subject to

$$F_s = \sum_{tu} F_{s,tu}, \quad \forall s \in S \tag{2.13}$$

$$\sum_{tu} F_{s,tu} + \sum_{tu'} F^{rec}_{tu',tu} = F^{in}_{tu}, \quad \forall tu \in TU \tag{2.14}$$

$$F^{in}_{tu} = F^{out}_{tu}, \quad \forall tu \in TU \tag{2.15}$$

$$F^{out}_{tu} = \sum_{tu'} F^{rec}_{tu,tu'} + F^{exit}_{tu}, \quad \forall tu \in TU \tag{2.16}$$

$$\sum_{tu} F^{exit}_{tu} = F^{final} \tag{2.17}$$

$$\sum_{s} F_{s,tu} C_{s,c} + \sum_{tu'} W^{rec}_{tu',tu,c} = W^{in}_{tu,c}, \quad \forall tu \in TU, c \in C \tag{2.18}$$

$$W^{rec}_{tu',tu,c} \geq \underline{F^{rec}_{tu',tu}} C^{out}_{tu',c} + F^{rec}_{tu',tu} \underline{C^{out}_{tu',c}} - \underline{F^{rec}_{tu',tu}}\,\underline{C^{out}_{tu',c}}, \quad \forall tu, tu' \in TU, c \in C \tag{2.19a}$$

$$W^{rec}_{tu',tu,c} \geq \overline{F^{rec}_{tu',tu}} C^{out}_{tu',c} + F^{rec}_{tu',tu} \overline{C^{out}_{tu',c}} - \overline{F^{rec}_{tu',tu}}\,\overline{C^{out}_{tu',c}}, \quad \forall tu, tu' \in TU, c \in C \tag{2.19b}$$

$$W^{rec}_{tu',tu,c} \leq \underline{F^{rec}_{tu',tu}} C^{out}_{tu',c} + F^{rec}_{tu',tu} \overline{C^{out}_{tu',c}} - \underline{F^{rec}_{tu',tu}}\,\overline{C^{out}_{tu',c}}, \quad \forall tu, tu' \in TU, c \in C \tag{2.19c}$$

$$W^{rec}_{tu',tu,c} \leq \overline{F^{rec}_{tu',tu}} C^{out}_{tu',c} + F^{rec}_{tu',tu} \underline{C^{out}_{tu',c}} - \overline{F^{rec}_{tu',tu}}\,\underline{C^{out}_{tu',c}}, \quad \forall tu, tu' \in TU, c \in C \tag{2.19d}$$

$$W^{in}_{tu,c} \geq \underline{F^{in}_{tu}} C^{in}_{tu,c} + F^{in}_{tu} \underline{C^{in}_{tu,c}} - \underline{F^{in}_{tu}}\,\underline{C^{in}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.20a}$$

$$W^{in}_{tu,c} \geq \overline{F^{in}_{tu}} C^{in}_{tu,c} + F^{in}_{tu} \overline{C^{in}_{tu,c}} - \overline{F^{in}_{tu}}\,\overline{C^{in}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.20b}$$

$$W^{in}_{tu,c} \leq \underline{F^{in}_{tu}} C^{in}_{tu,c} + F^{in}_{tu} \overline{C^{in}_{tu,c}} - \underline{F^{in}_{tu}}\,\overline{C^{in}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.20c}$$

$$W^{in}_{tu,c} \leq \overline{F^{in}_{tu}} C^{in}_{tu,c} + F^{in}_{tu} \underline{C^{in}_{tu,c}} - \overline{F^{in}_{tu}}\,\underline{C^{in}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.20d}$$

$$W^{in}_{tu,c} = W^{out}_{tu,c} + W^{in}_{tu,c} RR_{tu,c}, \quad \forall tu \in TU, c \in C \tag{2.21}$$

$$W^{out}_{tu,c} = \sum_{tu'} W^{rec}_{tu',tu,c} + W^{exit}_{tu,c}, \quad \forall tu \in TU, c \in C \tag{2.22}$$

$$W^{out}_{tu,c} \geq \underline{F^{out}_{tu}} C^{out}_{tu,c} + F^{out}_{tu} \underline{C^{out}_{tu,c}} - \underline{F^{out}_{tu}}\,\underline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.23a}$$

$$W^{out}_{tu,c} \geq \overline{F^{out}_{tu}} C^{out}_{tu,c} + F^{out}_{tu} \overline{C^{out}_{tu,c}} - \overline{F^{out}_{tu}}\,\overline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.23b}$$

$$W^{out}_{tu,c} \leq \underline{F^{out}_{tu}} C^{out}_{tu,c} + F^{out}_{tu} \overline{C^{out}_{tu,c}} - \underline{F^{out}_{tu}}\,\overline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.23c}$$

$$W^{out}_{tu,c} \leq \overline{F^{out}_{tu}} C^{out}_{tu,c} + F^{out}_{tu} \underline{C^{out}_{tu,c}} - \overline{F^{out}_{tu}}\,\underline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.23d}$$

$$\sum_{tu} W^{exit}_{tu,c} = W^{final}_{c}, \quad \forall c \in C \tag{2.24}$$

$$W^{exit}_{tu,c} \geq \underline{F^{exit}_{tu}} C^{out}_{tu,c} + F^{exit}_{tu} \underline{C^{out}_{tu,c}} - \underline{F^{exit}_{tu}}\,\underline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.25a}$$

$$W^{exit}_{tu,c} \geq \overline{F^{exit}_{tu}} C^{out}_{tu,c} + F^{exit}_{tu} \overline{C^{out}_{tu,c}} - \overline{F^{exit}_{tu}}\,\overline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.25b}$$

$$W^{exit}_{tu,c} \leq \underline{F^{exit}_{tu}} C^{out}_{tu,c} + F^{exit}_{tu} \overline{C^{out}_{tu,c}} - \underline{F^{exit}_{tu}}\,\overline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.25c}$$

$$W^{exit}_{tu,c} \leq \overline{F^{exit}_{tu}} C^{out}_{tu,c} + F^{exit}_{tu} \underline{C^{out}_{tu,c}} - \overline{F^{exit}_{tu}}\,\underline{C^{out}_{tu,c}}, \quad \forall tu \in TU, c \in C \tag{2.25d}$$

$$W^{final}_{c} \geq \underline{F^{final}} C^{final}_{c} + F^{final} \underline{C^{final}_{c}} - \underline{F^{final}}\,\underline{C^{final}_{c}}, \quad \forall c \in C \tag{2.26a}$$

$$W^{final}_{c} \geq \overline{F^{final}} C^{final}_{c} + F^{final} \overline{C^{final}_{c}} - \overline{F^{final}}\,\overline{C^{final}_{c}}, \quad \forall c \in C \tag{2.26b}$$

$$W_c^{final} \leq \underline{F^{final}} C_c^{final} + F^{final} \overline{C_c^{final}} - \underline{F^{final}}\,\overline{C_c^{final}}, \quad \forall c \in C \tag{2.26c}$$

$$W_c^{final} \leq \overline{F^{final}} C_c^{final} + F^{final} \underline{C_c^{final}} - \overline{F^{final}}\,\underline{C_c^{final}}, \quad \forall c \in C \tag{2.26d}$$

$$C_c^{\text{final}} \leq C_c^{\text{target}}, \quad \forall c \in C \tag{2.27}$$

Table 2.3: Bounding values for variables involved in bilinear terms in the McCormick relaxation of the small water treatment model

| Variable | Lower limit | Upper limit |
|---|---|---|
| $F_{tu',tu}^{rec}$ | 0 | $\sum_s F_s$ |
| $F_{tu}^{in}$ | 0 | $\sum_s F_s$ |
| $F_{tu}^{out}$ | 0 | $\sum_s F_s$ |
| $F_{tu}^{exit}$ | 0 | $\sum_s F_s$ |
| $F^{final}$ | 0 | $\sum_s F_s$ |
| $C_{tu,c}^{in}$ | 0 | $\max_s C_{s,c}$ |
| $C_{tu,c}^{out}$ | 0 | $\max_s C_{s,c}$ |
| $C_c^{final}$ | 0 | $\max_s C_{s,c}$ |

The relaxed LP model was solved on GAMS using the CPLEX LP solver. The locally optimal objective magnitude at nominal conditions was found to be 80.9836 tonne/hr, and the resulting optimal network is shown in Figure 2.3.

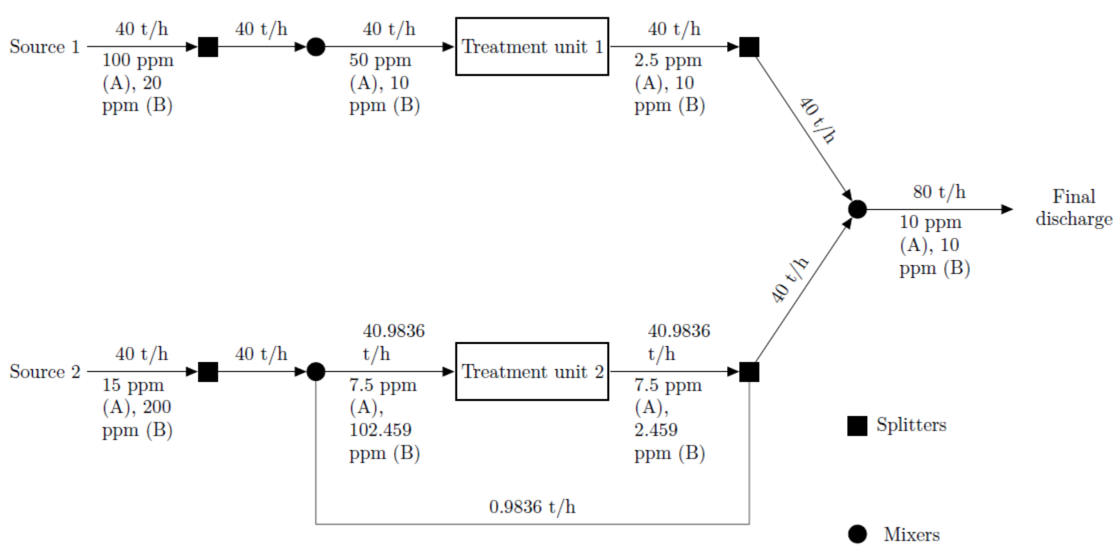


Figure 2.3: Optimal solution for the relaxed LP formulation of the small water treatment model

## 2.5 Robust counterpart of the stochastic LDR formulation using the relaxed LP model

The general optimization problem under uncertainty can be solved by a variety of methods. A survey of these methods is presented in Section 1.6 of this thesis. The aim of this thesis was the application of a specific stochastic programming solution technique - the class of decision rule-based methods - to obtain an adaptive solution to the general nonlinear model. The simplest configuration of these decision rule-based methods utilizes the affine decision rule, usually referred to as the linear decision rule (LDR). The procedure to obtain the adjustable affine robust counterpart of a constraint linear in uncertainty is detailed in Section 1.6.4.

The LDR formulation was applied to the flow, concentration and bilinear substitute variables ($W$). In this problem, the source flow $F_s$ was assumed to be the uncertain parameter, depending on primitive uncertainty $\xi$ as follows,

$$F_s(\xi) = \xi F_s^1 + (1-\xi)F_s^2, \quad \forall s \in S$$

where $F_s^1$ and $F_s^2$ were taken to be the extreme points for the realizations of $F_s$. For all LDR-based formulations involving the small water treatment model in this thesis, the source flow was assumed to vary between 25 tonne/hr ($F_s^1$) and 55 tonne/hr ($F_s^2$).

The tractable robust counterpart to the stochastic problem using the affine decision rule was modeled as follows, using the relaxed LP formulation in Section 2.4, for different ranges of uncertainty $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$. In this model, $\gamma$ and $\alpha$ refer to the dual variables associated with the McCormick envelope constraints and non-negativity constraints respectively, while $\lambda_c$ refers to the dual variables associated with the target concentration constraints. The sets of decision rule parameters optimized by this model are depicted by $F^0$ and $F^1$ for flow variables, $C^0$ and $C^1$ for concentration variables, and $W^0$ and $W^1$ for substitute variables.

$$\min \quad \sum_{tu} F_{tu}^{in,0} + F_{tu}^{in,1} E[\xi] \tag{2.28}$$

subject to

$$F_s^2 - \sum_{tu} F_{s,tu}^0 = 0, \quad s \in S \tag{2.29a}$$

$$F_s^1 - F_s^2 - \sum_{tu} F_{s,tu}^1 = 0, \quad s \in S \tag{2.29b}$$

$$\sum_{s} F^{0}_{s,tu} + \sum_{tu'} F^{rec,0}_{tu',tu} - F^{in,0}_{tu} = 0, \quad tu \in TU \tag{2.30a}$$

$$\sum_{s} F^{1}_{s,tu} + \sum_{tu'} F^{rec,1}_{tu',tu} - F^{in,1}_{tu} = 0, \quad tu \in TU \tag{2.30b}$$

$$F^{in,0}_{tu} - F^{out,0}_{tu} = 0, \quad tu \in TU \tag{2.31a}$$

$$F^{in,1}_{tu} - F^{out,1}_{tu} = 0, \quad tu \in TU \tag{2.31b}$$

$$F^{out,0}_{tu} - \sum_{tu'} F^{rec,0}_{tu,tu'} - F^{exit,0}_{tu} = 0, \quad tu \in TU \tag{2.32a}$$

$$F^{out,1}_{tu} - \sum_{tu'} F^{rec,1}_{tu,tu'} - F^{exit,1}_{tu} = 0, \quad tu \in TU \tag{2.32b}$$

$$\sum_{tu} F^{exit,0}_{tu} - F^{final,0} = 0 \tag{2.33a}$$

$$\sum_{tu} F^{exit,1}_{tu} - F^{final,1} = 0 \tag{2.33b}$$

$$\sum_{s} F^{0}_{s,tu} C_{s,c} + \sum_{tu'} W^{rec,0}_{tu',tu,c} - W^{in,0}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.34a}$$

$$\sum_{s} F^{1}_{s,tu} C_{s,c} + \sum_{tu'} W^{rec,1}_{tu',tu,c} - W^{in,1}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.34b}$$

$$W^{in,0}_{tu,c}(1 - RR_{tu,c}) - W^{out,0}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.35a}$$

$$W^{in,1}_{tu,c}(1 - RR_{tu,c}) - W^{out,1}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.35b}$$

$$W^{out,0}_{tu,c} - \sum_{tu'} W^{rec,0}_{tu,tu',c} - W^{exit,0}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.36a}$$

$$W^{out,1}_{tu,c} - \sum_{tu'} W^{rec,1}_{tu,tu',c} - W^{exit,1}_{tu,c} = 0, \quad tu \in TU, c \in C \tag{2.36b}$$

$$\sum_{tu} W^{exit,0}_{tu,c} - W^{final,0}_{c} = 0, \quad c \in C \tag{2.37a}$$

$$\sum_{tu} W^{exit,1}_{tu,c} - W^{final,1}_{c} = 0, \quad c \in C \tag{2.37b}$$

$$(C^{target}_{c} - C^{final,0}_{c}) + b^{\top}\lambda_c \geq 0, \quad c \in C \tag{2.38a}$$

$$A^{\top}\lambda_c + C^{final,1}_{c} = 0, \quad c \in C \tag{2.38b}$$

$$\begin{aligned} W^{rec,0}_{tu',tu,c} + \underline{F^{rec}_{tu',tu} C^{out}_{tu,c}} - \underline{F^{rec}_{tu',tu}} C^{out,0}_{tu,c} \\ - \underline{C^{out}_{tu,c}} F^{rec,0}_{tu',tu} + b^{\top}\gamma^{ll,1}_{tu',tu,c} \geq 0, \quad tu', tu \in TU, c \in C \end{aligned} \tag{2.39a}$$

$$A^{\top}\gamma^{ll,1}_{tu',tu,c} = W^{rec,1}_{tu',tu,c} - \underline{F^{rec}_{tu',tu}} C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}} F^{rec,1}_{tu',tu}, \quad tu', tu \in TU, c \in C \tag{2.39b}$$

$$W^{in,0}_{tu,c} + \underline{F^{in}_{tu} C^{in}_{tu,c}} - \underline{F^{in}_{tu}} C^{in,0}_{tu,c} - \underline{C^{in}_{tu,c}} F^{in,0}_{tu} + b^\top \gamma^{ll,2}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.40a}$$

$$A^\top \gamma^{ll,2}_{tu,c} = W^{in,1}_{tu,c} - \underline{F^{in}_{tu}} C^{in,1}_{tu,c} - \underline{C^{in}_{tu,c}} F^{in,1}_{tu}, \quad tu \in TU, c \in C \tag{2.40b}$$

$$W^{out,0}_{tu,c} + \underline{F^{out}_{tu} C^{out}_{tu,c}} - \underline{F^{out}_{tu}} C^{out,0}_{tu,c} - \underline{C^{out}_{tu,c}} F^{out,0}_{tu} + b^\top \gamma^{ll,3}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.41a}$$

$$A^\top \gamma^{ll,3}_{tu,c} = W^{out,1}_{tu,c} - \underline{F^{out}_{tu}} C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}} F^{out,1}_{tu}, \quad tu \in TU, c \in C \tag{2.41b}$$

$$W^{exit,0}_{tu,c} + \underline{F^{exit}_{tu} C^{out}_{tu,c}} - \underline{F^{exit}_{tu}} C^{out,0}_{tu,c} - \underline{C^{out}_{tu,c}} F^{exit,0}_{tu} + b^\top \gamma^{ll,4}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.42a}$$

$$A^\top \gamma^{ll,4}_{tu,c} = W^{exit,1}_{tu,c} - \underline{F^{exit}_{tu}} C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}} F^{exit,1}_{tu}, \quad tu \in TU, c \in C \tag{2.42b}$$

$$W^{final,0}_{c} + \underline{F^{final} C^{final}_{c}} - \underline{F^{final}} C^{final,0}_{c} - \underline{C^{final}_{c}} F^{final,0} + b^\top \gamma^{ll,5}_{c} \geq 0, \quad c \in C \tag{2.43a}$$

$$A^\top \gamma^{ll,5}_{c} = W^{final,1}_{c} - \underline{F^{final}} C^{final,1}_{c} - \underline{C^{final}_{c}} F^{final,1}, \quad c \in C \tag{2.43b}$$

$$W^{rec,0}_{tu',tu,c} + \overline{F^{rec}_{tu',tu} C^{out}_{tu,c}} - \overline{F^{rec}_{tu',tu}} C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}} F^{rec,0}_{tu',tu} + b^\top \gamma^{uu,1}_{tu',tu,c} \geq 0, \quad tu', tu \in TU, c \in C \tag{2.44a}$$

$$A^\top \gamma^{uu,1}_{tu',tu,c} = W^{rec,1}_{tu',tu,c} - \overline{F^{rec}_{tu',tu}} C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}} F^{rec,1}_{tu',tu}, \quad tu', tu \in TU, c \in C \tag{2.44b}$$

$$W^{in,0}_{tu,c} + \overline{F^{in}_{tu} C^{in}_{tu,c}} - \overline{F^{in}_{tu}} C^{in,0}_{tu,c} - \overline{C^{in}_{tu,c}} F^{in,0}_{tu} + b^\top \gamma^{uu,2}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.45a}$$

$$A^\top \gamma^{uu,2}_{tu,c} = W^{in,1}_{tu,c} - \overline{F^{in}_{tu}} C^{in,1}_{tu,c} - \overline{C^{in}_{tu,c}} F^{in,1}_{tu}, \quad tu \in TU, c \in C \tag{2.45b}$$

$$W^{out,0}_{tu,c} + \overline{F^{out}_{tu} C^{out}_{tu,c}} - \overline{F^{out}_{tu}} C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}} F^{out,0}_{tu} + b^\top \gamma^{uu,3}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.46a}$$

$$A^\top \gamma^{uu,3}_{tu,c} = W^{out,1}_{tu,c} - \overline{F^{out}_{tu}} C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}} F^{out,1}_{tu}, \quad tu \in TU, c \in C \tag{2.46b}$$

$$W^{exit,0}_{tu,c} + \overline{F^{exit}_{tu} C^{out}_{tu,c}} - \overline{F^{exit}_{tu}} C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}} F^{exit,0}_{tu} + b^\top \gamma^{uu,4}_{tu,c} \geq 0, \quad tu \in TU, c \in C \tag{2.47a}$$

$$A^\top \gamma^{uu,4}_{tu,c} = W^{exit,1}_{tu,c} - \overline{F^{exit}_{tu}} C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}} F^{exit,1}_{tu}, \quad tu \in TU, c \in C \tag{2.47b}$$

$$W^{final,0}_{c} + \overline{F^{final} C^{final}_{c}} - \overline{F^{final}} C^{final,0}_{c} - \overline{C^{final}_{c}} F^{final,0} + b^\top \gamma^{uu,5}_{c} \geq 0, \quad c \in C \tag{2.48a}$$

$$A^\top \gamma^{uu,5}_{c} = W^{final,1}_{c} - \overline{F^{final}} C^{final,1}_{c} - \overline{C^{final}_{c}} F^{final,1}, \quad c \in C \tag{2.48b}$$

$$W^{rec,0}_{tu',tu,c} + \underline{F^{rec}_{tu',tu}} \overline{C^{out}_{tu,c}} - \underline{F^{rec}_{tu',tu}} C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}} F^{rec,0}_{tu',tu} + b^\top \gamma^{lu,1}_{tu',tu,c} \leq 0, \quad tu', tu \in TU, c \in C \tag{2.49a}$$

$$A^\top \gamma^{lu,1}_{tu',tu,c} = W^{rec,1}_{tu',tu,c} - \underline{F^{rec}_{tu',tu}} C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}} F^{rec,1}_{tu',tu}, \quad tu', tu \in TU, c \in C \tag{2.49b}$$

$$W^{in,0}_{tu,c} + \underline{F^{in}_{tu}}\,\overline{C^{in}_{tu,c}} - \underline{F^{in}_{tu}}\,C^{in,0}_{tu,c} - \overline{C^{in}_{tu,c}}\,F^{in,0}_{tu} + b^\top \gamma^{lu,2}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.50a}$$

$$A^\top \gamma^{lu,2}_{tu,c} = W^{in,1}_{tu,c} - \underline{F^{in}_{tu}}\,C^{in,1}_{tu,c} - \overline{C^{in}_{tu,c}}\,F^{in,1}_{tu}, \quad tu \in TU, c \in C \tag{2.50b}$$

$$W^{out,0}_{tu,c} + \underline{F^{out}_{tu}}\,\overline{C^{out}_{tu,c}} - \underline{F^{out}_{tu}}\,C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}}\,F^{out,0}_{tu} + b^\top \gamma^{lu,3}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.51a}$$

$$A^\top \gamma^{lu,3}_{tu,c} = W^{out,1}_{tu,c} - \underline{F^{out}_{tu}}\,C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}}\,F^{out,1}_{tu}, \quad tu \in TU, c \in C \tag{2.51b}$$

$$W^{exit,0}_{tu,c} + \underline{F^{exit}_{tu}}\,\overline{C^{out}_{tu,c}} - \underline{F^{exit}_{tu}}\,C^{out,0}_{tu,c} - \overline{C^{out}_{tu,c}}\,F^{exit,0}_{tu} + b^\top \gamma^{lu,4}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.52a}$$

$$A^\top \gamma^{lu,4}_{tu,c} = W^{exit,1}_{tu,c} - \underline{F^{exit}_{tu}}\,C^{out,1}_{tu,c} - \overline{C^{out}_{tu,c}}\,F^{exit,1}_{tu}, \quad tu \in TU, c \in C \tag{2.52b}$$

$$W^{final,0}_{c} + \underline{F^{final}}\,\overline{C^{final}_{c}} - \underline{F^{final}}\,C^{final,0}_{c} - \overline{C^{final}_{c}}\,F^{final,0} + b^\top \gamma^{lu,5}_{c} \le 0, \quad c \in C \tag{2.53a}$$

$$A^\top \gamma^{lu,5}_{c} = W^{final,1}_{c} - \underline{F^{final}}\,C^{final,1}_{c} - \overline{C^{final}_{c}}\,F^{final,1}, \quad c \in C \tag{2.53b}$$

$$W^{rec,0}_{tu',tu,c} + \overline{F^{rec}_{tu',tu}}\,\underline{C^{out}_{tu,c}} - \overline{F^{rec}_{tu',tu}}\,C^{out,0}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{rec,0}_{tu',tu} + b^\top \gamma^{ul,1}_{tu',tu,c} \le 0, \quad tu', tu \in TU, c \in C \tag{2.54a}$$

$$A^\top \gamma^{ul,1}_{tu',tu,c} = W^{rec,1}_{tu',tu,c} - \overline{F^{rec}_{tu',tu}}\,C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{rec,1}_{tu',tu}, \quad tu', tu \in TU, c \in C \tag{2.54b}$$

$$W^{in,0}_{tu,c} + \overline{F^{in}_{tu}}\,\underline{C^{in}_{tu,c}} - \overline{F^{in}_{tu}}\,C^{in,0}_{tu,c} - \underline{C^{in}_{tu,c}}\,F^{in,0}_{tu} + b^\top \gamma^{ul,2}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.55a}$$

$$A^\top \gamma^{ul,2}_{tu,c} = W^{in,1}_{tu,c} - \overline{F^{in}_{tu}}\,C^{in,1}_{tu,c} - \underline{C^{in}_{tu,c}}\,F^{in,1}_{tu}, \quad tu \in TU, c \in C \tag{2.55b}$$

$$W^{out,0}_{tu,c} + \overline{F^{out}_{tu}}\,\underline{C^{out}_{tu,c}} - \overline{F^{out}_{tu}}\,C^{out,0}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{out,0}_{tu} + b^\top \gamma^{ul,3}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.56a}$$

$$A^\top \gamma^{ul,3}_{tu,c} = W^{out,1}_{tu,c} - \overline{F^{out}_{tu}}\,C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{out,1}_{tu}, \quad tu \in TU, c \in C \tag{2.56b}$$

$$W^{exit,0}_{tu,c} + \overline{F^{exit}_{tu}}\,\underline{C^{out}_{tu,c}} - \overline{F^{exit}_{tu}}\,C^{out,0}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{exit,0}_{tu} + b^\top \gamma^{ul,4}_{tu,c} \le 0, \quad tu \in TU, c \in C \tag{2.57a}$$

$$A^\top \gamma^{ul,4}_{tu,c} = W^{exit,1}_{tu,c} - \overline{F^{exit}_{tu}}\,C^{out,1}_{tu,c} - \underline{C^{out}_{tu,c}}\,F^{exit,1}_{tu}, \quad tu \in TU, c \in C \tag{2.57b}$$

$$W^{final,0}_{c} + \overline{F^{final}}\,\underline{C^{final}_{c}} - \overline{F^{final}}\,C^{final,0}_{c} - \underline{C^{final}_{c}}\,F^{final,0} + b^\top \gamma^{ul,5}_{c} \le 0, \quad c \in C \tag{2.58a}$$

$$A^\top \gamma^{ul,5}_{c} = W^{final,1}_{c} - \overline{F^{final}}\,C^{final,1}_{c} - \underline{C^{final}_{c}}\,F^{final,1}, \quad c \in C \tag{2.58b}$$

$$F^{0}_{s,tu} + b^\top \alpha^{F_{s,tu}}_{s,tu} \ge 0, \quad s \in S, tu \in TU \tag{2.59a}$$

$$A^\top \alpha^{F_{s,tu}}_{s,tu} = F^{1}_{s,tu}, \quad s \in S, tu \in TU \tag{2.59b}$$

$$F^{rec,0}_{tu',tu} + b^\top \alpha^{F^{rec}_{tu',tu}}_{tu',tu} \ge 0, \quad tu', tu \in TU \tag{2.60a}$$

$$A^\top \alpha^{F^{rec}_{tu',tu}}_{tu',tu} = F^{rec,1}_{tu',tu}, \quad tu', tu \in TU \tag{2.60b}$$

$$F_{tu}^{in,0} + b^\top \alpha_{tu}^{F_{tu}^{in}} \geq 0, \quad tu \in TU \tag{2.61a}$$
$$A^\top \alpha_{tu}^{F_{tu}^{in}} = F_{tu}^{in,1}, \quad tu \in TU \tag{2.61b}$$

$$F_{tu}^{out,0} + b^\top \alpha_{tu}^{F_{tu}^{out}} \geq 0, \quad tu \in TU \tag{2.62a}$$
$$A^\top \alpha_{tu}^{F_{tu}^{out}} = F_{tu}^{out,1}, \quad tu \in TU \tag{2.62b}$$

$$F_{tu}^{exit,0} + b^\top \alpha_{tu}^{F_{tu}^{exit}} \geq 0, \quad tu \in TU \tag{2.63a}$$
$$A^\top \alpha_{tu}^{F_{tu}^{exit}} = F_{tu}^{exit,1}, \quad tu \in TU \tag{2.63b}$$

$$F^{final,0} + b^\top \alpha^{F^{final}} \geq 0 \tag{2.64a}$$
$$A^\top \alpha^{F^{final}} = F^{final,1} \tag{2.64b}$$

$$C_{tu,c}^{in,0} + b^\top \alpha_{tu,c}^{C_{tu,c}^{in}} \geq 0, \quad tu \in TU, c \in C \tag{2.65a}$$
$$A^\top \alpha_{tu,c}^{C_{tu,c}^{in}} = C_{tu,c}^{in,1}, \quad tu \in TU, c \in C \tag{2.65b}$$

$$C_{tu,c}^{out,0} + b^\top \alpha_{tu,c}^{C_{tu,c}^{out}} \geq 0, \quad tu \in TU, c \in C \tag{2.66a}$$
$$A^\top \alpha_{tu,c}^{C_{tu,c}^{out}} = C_{tu,c}^{out,1}, \quad tu \in TU, c \in C \tag{2.66b}$$

$$C_c^{final,0} + b^\top \alpha_c^{C_c^{final}} \geq 0, \quad c \in C \tag{2.67a}$$
$$A^\top \alpha_c^{C_c^{final}} = C_c^{final,1}, \quad c \in C \tag{2.67b}$$

$$W_{tu',tu,c}^{rec,0} + b^\top \alpha_{tu',tu,c}^{W_{tu',tu,c}^{rec}} \geq 0, \quad tu', tu \in TU, c \in C \tag{2.68a}$$
$$A^\top \alpha_{tu',tu,c}^{W_{tu',tu,c}^{rec}} = W_{tu',tu,c}^{rec,1}, \quad tu', tu \in TU, c \in C \tag{2.68b}$$

$$W_{tu,c}^{in,0} + b^\top \alpha_{tu,c}^{W_{tu,c}^{in}} \geq 0, \quad tu \in TU, c \in C \tag{2.69a}$$
$$A^\top \alpha_{tu,c}^{W_{tu,c}^{in}} = W_{tu,c}^{in,1}, \quad tu \in TU, c \in C \tag{2.69b}$$

$$W_{tu,c}^{out,0} + b^\top \alpha_{tu,c}^{W_{tu,c}^{out}} \geq 0, \quad tu \in TU, c \in C \tag{2.70a}$$
$$A^\top \alpha_{tu,c}^{W_{tu,c}^{out}} = W_{tu,c}^{out,1}, \quad tu \in TU, c \in C \tag{2.70b}$$

$$W_{tu,c}^{exit,0} + b^\top \alpha_{tu,c}^{W_{tu,c}^{exit}} \geq 0, \quad tu \in TU, c \in C \tag{2.71a}$$
$$A^\top \alpha_{tu,c}^{W_{tu,c}^{exit}} = W_{tu,c}^{exit,1}, \quad tu \in TU, c \in C \tag{2.71b}$$

$$W_c^{final,0} + b^\top \alpha_c^{W_c^{final}} \geq 0, \quad c \in C \tag{2.72a}$$
$$A^\top \alpha_c^{W_c^{final}} = W_c^{final,1}, \quad c \in C \tag{2.72b}$$

The stochastic model using the LDR formulation on the relaxed LP model was solved using the CPLEX LP solver, and the locally optimal objective magnitude for $E[\xi] =$

0.5 was found to be 80 tonne/hr. The resulting optimal network is depicted for $\xi = 0.53$, using the LDR solution for $\xi \in [0.4, 0.6]$ in Figure 2.4 and $\xi \in [0, 1]$ in Figure 2.5. The optimal decision rule parameters for the variables in the model are given in Table 2.4. It was observed that the solution satisfied all flow balance equations in the model. However, neither the solution to the relaxed LP formulation nor the stochastic LDR model satisfied the original component balances in the model. It was inferred that the violation of component balances occurred as a consequence of replacing the bilinear terms with the new variables, and solving the model to satisfy these modified equations. In other words, the bilinear terms were merely replaced by the new variables, but no equivalence had been established between the entities. Therefore, the relaxed solution was deemed infeasible due to component balance violations throughout the model. This infeasibility was found to propagate into the stochastic LDR model as well, and hence, the optimal decision rules obtained from the stochastic LDR model were deemed infeasible.

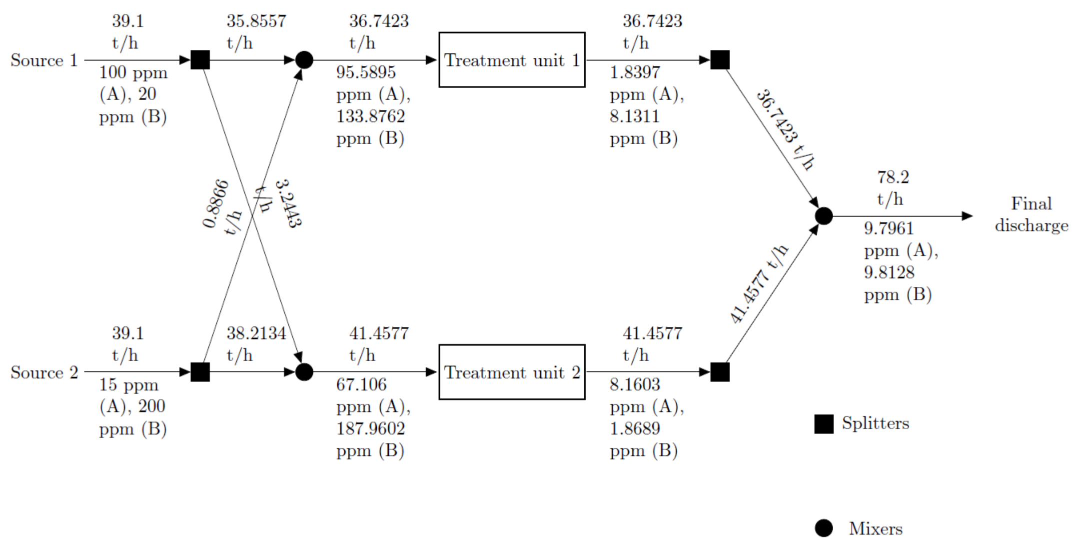


Figure 2.4: Optimal solution for the stochastic relaxed LDR formulation of the relaxed small water treatment model for $\xi \in [0.4, 0.6]$ at $\xi^* = 0.53$

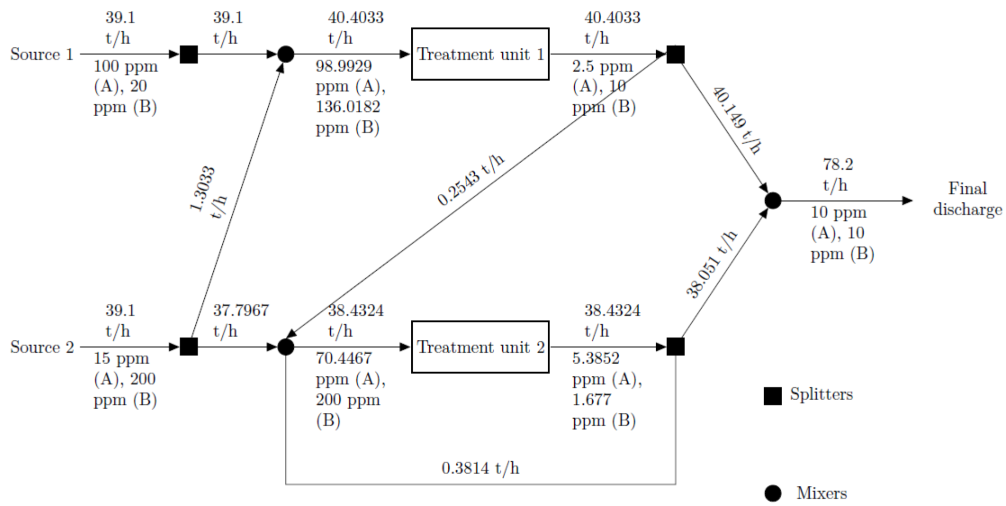


Figure 2.5: Optimal solution for the stochastic relaxed LDR formulation of the relaxed small water treatment model for $\xi \in [0, 1]$ at $\xi^* = 0.53$

Table 2.4: Decision rule parameters for the variables in the stochastic LDR formulation of the relaxed small water treatment model

| | $\xi \in [0.4, 0.6]$ | $\xi \in [0, 1]$ |
|---|---|---|
| $F_{s_1,tu_1}$ | 54.4192 - 35.0254$\xi$ | 55 - 30$\xi$ |
| $F_{s_1,tu_2}$ | 0.5808 + 5.0254$\xi$ | |
| $F_{s_2,tu_1}$ | -0.9698 + 3.5025$\xi$ | 2.459$\xi$ |
| $F_{s_2,tu_2}$ | 55.9698 - 33.5025$\xi$ | 55 - 32.459$\xi$ |
| $F^{in}_{tu_1}$ | 53.4494 - 31.5228$\xi$ | 55 - 27.541$\xi$ |
| $F^{in}_{tu_2}$ | 56.5506 - 28.4772$\xi$ | 56.3525 - 33.8115$\xi$ |
| $F^{out}_{tu_1}$ | 53.4494 - 31.5228$\xi$ | 55 - 27.541$\xi$ |
| $F^{out}_{tu_2}$ | 56.5506 - 28.4772$\xi$ | 56.3525 - 33.8115$\xi$ |
| $F^{rec}_{tu_1,tu_2}$ | | 0.541 - 0.541$\xi$ |
| $F^{rec}_{tu_2,tu_2}$ | | 0.8115 - 0.8115$\xi$ |
| $F^{exit}_{tu_1}$ | 53.4494 - 31.5228$\xi$ | 54.459 - 27$\xi$ |
| $F^{exit}_{tu_2}$ | 56.5506 - 28.4772$\xi$ | 55.541 - 33$\xi$ |
| $F^{final}$ | 110 - 60$\xi$ | 110 - 60$\xi$ |
| $C^{in}_{tu_1,A}$ | 112.2122 - 31.3636$\xi$ | 100 - 1.9001$\xi$ |
| $C^{out}_{tu_1,A}$ | 1.8397 | 2.5 |
| $C^{in}_{tu_1,B}$ | 133.8762 | 110 + 49.0909$\xi$ |
| $C^{out}_{tu_1,B}$ | 8.1311 | 10 |
| $C^{in}_{tu_2,A}$ | 67.106 | 56.7623 + 25.8197$\xi$ |
| $C^{out}_{tu_2,A}$ | 8.1603 | 7.9918 - 4.918$\xi$ |
| $C^{in}_{tu_2,B}$ | 219.7602 | 200 |
| $C^{out}_{tu_2,B}$ | 1.8689 | 2.459 - 1.4754$\xi$ |
| $C^{final}_{A}$ | 10.6273 - 1.5682$\xi$ | 10 |
| $C^{final}_{B}$ | 10.576 - 1.44$\xi$ | 10 |
| $W^{in}_{tu_1,A}$ | 5427.3684 - 3450$\xi$ | 5500 - 2963.1148$\xi$ |
| $W^{out}_{tu_1,A}$ | 271.3684 - 172.5$\xi$ | 275 - 148.1557$\xi$ |
| $W^{in}_{tu_1,B}$ | 894.4262 | 1100 - 108.1967$\xi$ |
| $W^{out}_{tu_1,B}$ | 894.4262 | 1100 - 108.1967$\xi$ |
| $W^{in}_{tu_2,A}$ | 897.6316 | 879.0984 - 540.9836$\xi$ |
| $W^{out}_{tu_2,A}$ | 897.6136 | 879.0984 - 540.9836$\xi$ |
| $W^{in}_{tu_2,B}$ | 11205.5738 - 6600$\xi$ | 11270.4918 - 6762.2951$\xi$ |
| $W^{out}_{tu_2,B}$ | 268.9338 - 158.4$\xi$ | 270.4918 - 162.2951$\xi$ |
| $W^{rec}_{tu_1,tu_2,A}$ | | 54.0984 - 54.0984$\xi$ |
| $W^{rec}_{tu_1,tu_2,B}$ | | 108.1967 - 108.1967$\xi$ |
| $W^{rec}_{tu_2,tu_2,B}$ | | 162.2951 - 162.2951$\xi$ |
| $W^{exit}_{tu_1,A}$ | 271.3684 - 172.5$\xi$ | 220.9016 - 94.0574$\xi$ |
| $W^{exit}_{tu_1,B}$ | 894.4262 | 991.8033 |
| $W^{exit}_{tu_2,A}$ | 897.6316 | 879.0984 - 540.9836$\xi$ |
| $W^{exit}_{tu_2,B}$ | 268.9338 - 158.4$\xi$ | 108.1967 |
| $W^{final}_{A}$ | 1169 - 172.5$\xi$ | 1100 - 635.041$\xi$ |
| $W^{final}_{B}$ | 1163.36 - 158.4$\xi$ | 1100 |

## 2.6 Concluding remarks

This chapter presented the application of the affine decision rule-based stochastic optimization method on the relaxed LP formulation of the small water treatment model. The usage of McCormick envelopes for relaxation of a nonlinear model was discussed in Section 2.1, and its application on the small water treatment model was depicted in Section 2.4. The stochastic LDR-based formulation of the relaxed model under uncertainty was depicted in 2.5. It was observed that, due to inadequate linearization of the NLP model using McCormick envelopes, the decision rules obtained for the model variables lead to violation of the component balance constraints, thereby rendering the decision rules/policies infeasible for practical application.

# Chapter 3

# Linear Stochastic Optimization using Taylor Series Approximation

In this chapter, the application of the Taylor series approximation to the small water treatment NLP model is discussed. The model is linearized around the set of nominal operating conditions, using first order Taylor series approximation. Section 3.1 provides a brief background on linearization of functions using Taylor series, and Section 3.2 presents the solution of the linearized model. The derivation and solution of the stochastic LDR-based formulation of the relaxed LP model is presented and analyzed in Section 3.3.

## 3.1 Linearization using Taylor Series approximation

The Taylor series expansion of a function $f(x, y)$ may be defined as an approximation of the function using an infinite sum of terms or a polynomial. In most applications, taking only a finite number of terms into account proves sufficient to approximate the function; the higher the number of terms in the polynomial approximation, the smaller the error between the actual function and the approximation.

A Taylor series approximation of a function is constructed around a specific value of the function; this point is be denoted by $(x^*, y^*)$. As one moves away from $(x^*, y^*)$, the approximation of the function $f(x, y)$ is expected to get worse. The Taylor series of a function $f(x, y)$ around a value $(x^*, y^*)$ is given in Equation 3.1.

$$f(x,y) = f(x^*,y^*) + (x-x^*)\left.\frac{\partial f}{\partial x}\right|_{(x^*,y^*)} + (y-y^*)\left.\frac{\partial f}{\partial y}\right|_{(x^*,y^*)} + \frac{(x-x^*)^2}{2!}\left.\frac{\partial^2 f}{\partial x^2}\right|_{(x^*,y^*)}$$
$$+ \frac{(y-y^*)^2}{2!}\left.\frac{\partial^2 f}{\partial y^2}\right|_{(x^*,y^*)} + ... + \frac{(x-x^*)^n}{n!}\left.\frac{\partial^n f}{\partial x^n}\right|_{(x^*,y^*)} + \frac{(y-y^*)^n}{n!}\left.\frac{\partial^n f}{\partial y^n}\right|_{(x^*,y^*)} \quad (3.1)$$

In the deterministic formulation of the small water treatment model, the presence of bilinear terms in the component balance equations (2.7 - 2.10) makes the optimization exercise a nonlinear program (NLP). A linear approximation of the bilinear terms can be performed using first order Taylor series approximation around the set of nominal operating conditions, i.e, the operating values of the variables at $\xi^*$.

Let $F(\xi) \cdot C(\xi)$ be a bilinear term occurring in the small water treatment model. It can be approximated using first order Taylor series expansion, as follows.

$$F(\xi) \cdot C(\xi) \approx F(\xi^*)C(\xi^*) + [F(\xi) - F(\xi^*)]\frac{\partial}{\partial F}(F(\xi) \cdot C(\xi))\Big|_{\xi^*}$$
$$+[C(\xi) - C(\xi^*)]\frac{\partial}{\partial C}(F(\xi) \cdot C(\xi))\Big|_{\xi^*}$$

$$F(\xi) \cdot C(\xi) \approx F(\xi^*)C(\xi^*) + [F(\xi) - F(\xi^*)]C(\xi^*) + [C(\xi) - C(\xi^*)]F(\xi^*)$$

$$F(\xi) \cdot C(\xi) \approx F(\xi)C(\xi^*) + C(\xi)F(\xi^*) - F(\xi^*)C(\xi^*)$$

Applying the LDR formulation to the variables, the bilinear term can be further reformulated as follows:

$$F(\xi) \cdot C(\xi) \approx (F^0 + F^1\xi)C(\xi^*) + (C^0 + C^1\xi)F(\xi^*) - F(\xi^*)C(\xi^*)$$

$$F(\xi) \cdot C(\xi) \approx [F^0 C(\xi^*) + C^0 F(\xi^*) - F(\xi^*)C(\xi^*)] + \xi[F^1 C(\xi^*) + C^1 F(\xi^*)] \quad (3.2)$$

The bilinear terms in the stochastic formulation of the model described in Section 2.3 were replaced using the approximation in Equation 3.2. The robust counterpart to the equality constraints was obtained by equating the coefficients of $\xi$ to zero, while the counterpart to the inequality constraints was obtained using the technique detailed in Section 1.6.4.

In this chapter, the application of first order Taylor series approximation to obtain the linear counterpart of the component balances was studied in the context of obtaining the optimal solution and checking for feasibility, as well as its performance against the NLP solution.

## 3.2 Linearized formulation of the model

The first order Taylor series approximation was initially applied to the bilinear terms in the deterministic formulation of the small water treatment model given in Section 2.2. The model was linearized around the set of operating values of the variables at the nominal condition. These operating values were obtained from the optimal solution of the deterministic model corresponding to $\xi^* = 0.5$. The nominal operating conditions around which the model was linearized are given in Table 3.1.

$$\min \quad \sum_{tu} F_{tu}^{in} \tag{3.3}$$

subject to

$$F_s = \sum_{tu} F_{s,tu}, \quad \forall s \in S \tag{3.4}$$

$$\sum_s F_{s,tu} + \sum_{tu'} F_{tu',tu}^{rec} = F_{tu}^{in}, \quad \forall tu \in TU \tag{3.5}$$

$$F_{tu}^{in} = F_{tu}^{out}, \quad \forall tu \in TU \tag{3.6}$$

$$F_{tu}^{out} = \sum_{tu'} F_{tu,tu'}^{rec} + F_{tu}^{exit}, \quad \forall tu \in TU \tag{3.7}$$

$$\sum_{tu} F_{tu}^{exit} = F^{final} \tag{3.8}$$

$$\sum_s F_{s,tu} C_{s,c} + \sum_{tu'} F_{tu',tu}^{rec} C_{tu,c}^{out^*} + F_{tu',tu}^{rec^*} C_{tu,c}^{out} - F_{tu',tu}^{rec^*} C_{tu,c}^{out^*}$$
$$= F_{tu}^{in} C_{tu,c}^{in^*} + F_{tu}^{in^*} C_{tu,c}^{in} - F_{tu}^{in^*} C_{tu,c}^{in^*}, \quad \forall tu \in TU, c \in C \tag{3.9}$$

$$[F_{tu}^{in} C_{tu,c}^{in^*} + F_{tu}^{in^*} C_{tu,c}^{in} - F_{tu}^{in^*} C_{tu,c}^{in^*}](1 - RR_{tu,c})$$
$$= F_{tu}^{out} C_{tu,c}^{out^*} + F_{tu}^{out^*} C_{tu,c}^{out} - F_{tu}^{out^*} C_{tu,c}^{out^*}, \quad \forall tu \in TU, c \in C \tag{3.10}$$

$$F_{tu}^{out} C_{tu,c}^{out^*} + F_{tu}^{out^*} C_{tu,c}^{out} - F_{tu}^{out^*} C_{tu,c}^{out^*} = \sum_{tu'} F_{tu',tu}^{rec} C_{tu,c}^{out^*} + F_{tu',tu}^{rec^*} C_{tu,c}^{out} - F_{tu',tu}^{rec^*} C_{tu,c}^{out^*}$$
$$+ F_{tu}^{exit} C_{tu,c}^{out^*} + F_{tu}^{exit^*} C_{tu,c}^{out} - F_{tu}^{exit^*} C_{tu,c}^{out^*}, \quad \forall tu \in TU, c \in C \tag{3.11}$$

$$\sum_{tu} F_{tu}^{exit} C_{tu,c}^{out^*} + F_{tu}^{exit^*} C_{tu,c}^{out} - F_{tu}^{exit^*} C_{tu,c}^{out^*}$$
$$= F^{final} C_c^{final^*} + F^{final^*} C_c^{final} - F^{final^*} C_c^{final^*}, \quad \forall c \in C \tag{3.12}$$

$$C_c^{\text{final}} \leq C_c^{\text{target}}, \quad \forall c \in C \tag{3.13}$$

Table 3.1: Operating conditions for first order Taylor series approximation of the small water treatment model

| Flow variables (tonne/hr) | Value |
|---|---|
| $F^{*}_{s_1,tu_1}$ | 40 |
| $F^{*}_{s_2,tu_2}$ | 40 |
| $F^{in^*}_{tu_1}$ | 40 |
| $F^{in^*}_{tu_2}$ | 49.8361 |
| $F^{out^*}_{tu_1}$ | 40 |
| $F^{out^*}_{tu_2}$ | 49.8361 |
| $F^{rec^*}_{tu_1,tu_2}$ | 9.8361 |
| $F^{exit^*}_{tu_1}$ | 30.1639 |
| $F^{exit^*}_{tu_2}$ | 49.8361 |
| $F^{final^*}$ | 80 |
| **Concentration variables (ppm)** | **Value** |
| $C^{in^*}_{tu_1,A}$ | 100 |
| $C^{in^*}_{tu_1,B}$ | 20 |
| $C^{in^*}_{tu_2,A}$ | 13.0263 |
| $C^{in^*}_{tu_2,B}$ | 164.4737 |
| $C^{out^*}_{tu_1,A}$ | 5 |
| $C^{out^*}_{tu_1,B}$ | 20 |
| $C^{out^*}_{tu_2,A}$ | 13.0263 |
| $C^{out^*}_{tu_2,B}$ | 3.9474 |
| $C^{final^*}_{A}$ | 10 |
| $C^{final^*}_{B}$ | 10 |

The linearized model was solved on GAMS using the CPLEX LP solver. The optimal objective magnitude was found to be 116.6767 tonne/hr, and the resulting optimal network for the linearized model is depicted in Figure 3.1.

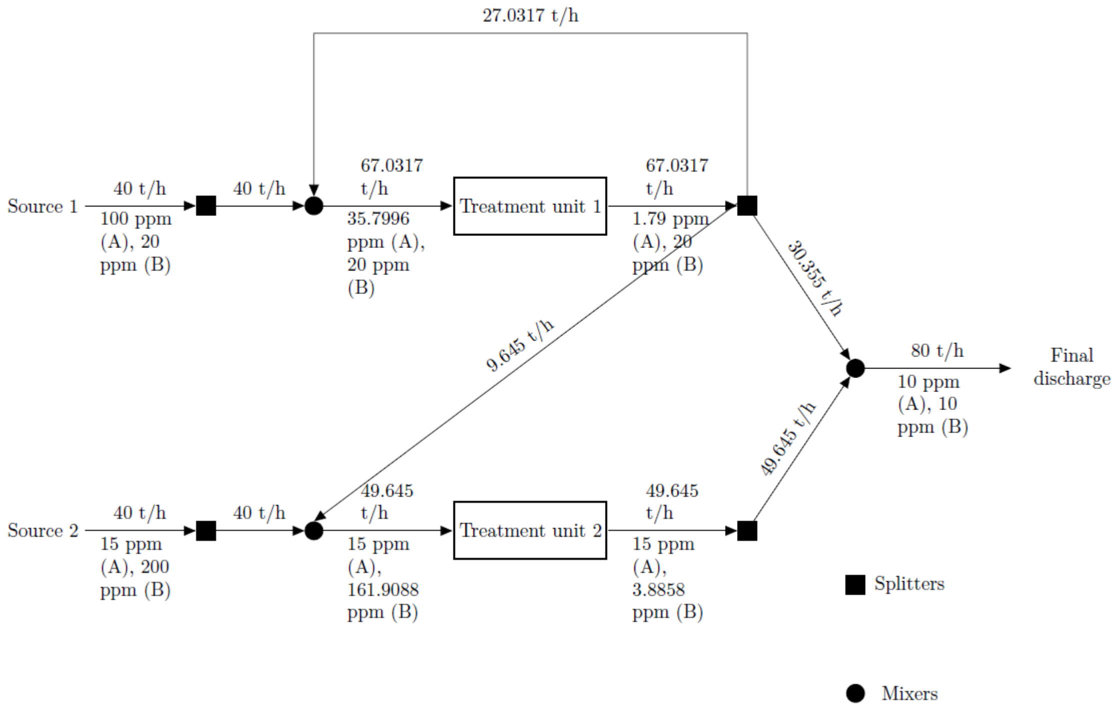


Figure 3.1: Optimal solution for the linearized formulation of the small water treatment model

## 3.3 Robust counterpart of the stochastic LDR formulation of the linearized model

The robust counterpart of the stochastic linearized formulation of the small water treatment model in Section 3.2 was obtained using the techniques detailed in Section 1.6.4. In this problem, the source flow $F_s$ was assumed to be the uncertain parameter, depending on primitive uncertainty $\xi$, as follows,

$$F_s(\xi) = \xi F_s^1 + (1-\xi)F_s^2, \quad \forall s \in S$$

where $F_s^1$ and $F_s^2$ were taken to be the extreme points for the realizations of $F_s$. The source flow was assumed to vary between 25 tonne/hr ($F_s^1$) and 55 tonne/hr ($F_s^2$).

Then, the finite tractable counterpart to the stochastic programming problem using the affine decision rule was modeled as follows, using the linearized model in Section 3.2, for different ranges of uncertainty. In this model, the variables $\lambda_c$ and $\alpha$ refer to the dual variables resulting from the robust counterpart of the concentration target constraint, and the non-negativity constraints, respectively. The sets of decision rule parameters optimized by this model are grouped into $F^0$ and $F^1$ for flow variables, and $C^0$ and $C^1$ for concentration variables.

$$\min \quad \sum_{tu} F_{tu}^{in,0} + F_{tu}^{in,1} E[\xi] \tag{3.14}$$

subject to

$$F_s^2 - \sum_{tu} F_{s,tu}^0 = 0, \quad s \in S \tag{3.15a}$$

$$F_s^1 - F_s^2 - \sum_{tu} F_{s,tu}^1 = 0, \quad s \in S \tag{3.15b}$$

$$\sum_s F_{s,tu}^0 + \sum_{tu'} F_{tu',tu}^{rec,0} - F_{tu}^{in,0} = 0, \quad tu \in TU \tag{3.16a}$$

$$\sum_s F_{s,tu}^1 + \sum_{tu'} F_{tu',tu}^{rec,1} - F_{tu}^{in,1} = 0, \quad tu \in TU \tag{3.16b}$$

$$F_{tu}^{in,0} - F_{tu}^{out,0} = 0, \quad tu \in TU \tag{3.17a}$$

$$F_{tu}^{in,1} - F_{tu}^{out,1} = 0, \quad tu \in TU \tag{3.17b}$$

$$F_{tu}^{out,0} - \sum_{tu'} F_{tu,tu'}^{rec,0} - F_{tu}^{exit,0} = 0, \quad tu \in TU \tag{3.18a}$$

$$F_{tu}^{out,1} - \sum_{tu'} F_{tu,tu'}^{rec,1} - F_{tu}^{exit,1} = 0, \quad tu \in TU \tag{3.18b}$$

$$\sum_{tu} F_{tu}^{exit,0} - F^{final,0} = 0 \tag{3.19a}$$

$$\sum_{tu} F_{tu}^{exit,1} - F^{final,1} = 0 \tag{3.19b}$$

$$\begin{aligned}(\sum_s F_{s,tu}^0 C_{s,c}) - (\sum_{tu'} F_{tu',tu}^{rec^*} C_{tu,c}^{out^*}) + F_{tu}^{in^*} C_{tu,c}^{in^*} + (\sum_{tu'} F_{tu',tu}^{rec,0} C_{tu,c}^{out^*} \\ + C_{tu,c}^{out,0} F_{tu',tu}^{rec^*}) - F_{tu}^{in,0} C_{tu,c}^{in^*} - F_{tu}^{in^*} C_{tu,c}^{in,0} = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{3.20a}$$

$$\begin{aligned}(\sum_s F_{s,tu}^1 C_{s,c}) + (\sum_{tu'} F_{tu',tu}^{rec,1} C_{tu,c}^{out^*} + F_{tu',tu}^{rec^*} C_{tu,c}^{out,1}) \\ - F_{tu}^{in,1} C_{tu,c}^{in^*} - F_{tu}^{in^*} C_{tu,c}^{in,1} = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{3.20b}$$

$$\begin{aligned}F_{tu}^{out^*} C_{tu,c}^{out^*} - F_{tu}^{out,0} C_{tu,c}^{out^*} - F_{tu}^{out^*} C_{tu,c}^{out,0} - (1 - RR_{tu,c})(F_{tu}^{in^*} C_{tu,c}^{in^*} + F_{tu}^{in,0} C_{tu,c}^{in^*} \\ + F_{tu}^{in^*} C_{tu,c}^{in,0}) = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{3.21a}$$

$$\begin{aligned}(1 - RR_{tu,c})(F_{tu}^{in,1} C_{tu,c}^{in^*} + F_{tu}^{in^*} C_{tu,c}^{in,1}) - F_{tu}^{out,1} C_{tu,c}^{out^*} \\ - F_{tu}^{out^*} C_{tu,c}^{out,1} = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{3.21b}$$

$$(\sum_{tu'} F^{rec^*}_{tu,tu'} C^{out^*}_{tu,c}) + F^{exit^*}_{tu} C^{out^*}_{tu,c} - F^{out^*}_{tu} C^{out^*}_{tu,c} + F^{out,0}_{tu} C^{out^*}_{tu,c} + F^{out^*}_{tu} C^{out,0}_{tu,c}$$
$$-(\sum_{tu'} F^{rec,0}_{tu,tu'} C^{out^*}_{tu,c} - F^{rec^*}_{tu,tu'} C^{out,0}_{tu,c}) - F^{exit,0}_{tu} C^{out^*}_{tu,c} - F^{exit^*}_{tu} C^{out,0}_{tu,c} = 0, \quad \forall tu \in TU, c \in C \tag{3.22a}$$

$$F^{out,1}_{tu} C^{out^*}_{tu,c} + F^{out^*}_{tu} C^{out,1}_{tu,c} - (\sum_{tu'} F^{rec,1}_{tu,tu'} C^{out^*}_{tu,c}$$
$$- F^{rec^*}_{tu,tu'} C^{out,1}_{tu,c}) - F^{exit,1}_{tu} C^{out^*}_{tu,c} - F^{exit^*}_{tu} C^{out,1}_{tu,c} = 0, \quad \forall tu \in TU, c \in C \tag{3.22b}$$

$$F^{final^*} C^{final^*}_{c} - (\sum_{tu} F^{exit^*}_{tu} C^{out^*}_{tu,c}) + (\sum_{tu} F^{exit,0}_{tu} C^{out^*}_{tu,c}$$
$$+ F^{exit^*}_{tu} C^{out,0}_{tu,c}) - F^{final,0} C^{final^*}_{c} - F^{final^*} C^{final,0}_{c} = 0, \quad \forall c \in C \tag{3.23a}$$

$$(\sum_{tu} F^{exit,1}_{tu} C^{out^*}_{tu,c} + F^{exit^*}_{tu} C^{out,1}_{tu,c}) - F^{final,1} C^{final^*}_{c} - F^{final^*} C^{final,1}_{c} = 0, \quad \forall c \in C \tag{3.23b}$$

$$(C^{target}_{c} - C^{final,0}_{c}) + b^\top \lambda_c \geq 0, \quad c \in C \tag{3.24a}$$
$$A^\top \lambda_c + C^{final,1}_{c} = 0, \quad c \in C \tag{3.24b}$$

$$F^{0}_{s,tu} + b^\top \alpha_{F_{s,tu}} \geq 0, \quad s \in S, tu \in TU \tag{3.25a}$$
$$A^\top \alpha_{F_{s,tu}} = F^{1}_{s,tu}, \quad s \in S, tu \in TU \tag{3.25b}$$

$$F^{rec,0}_{tu',tu} + b^\top \alpha_{F^{rec}_{tu',tu}} \geq 0, \quad tu', tu \in TU \tag{3.26a}$$
$$A^\top \alpha_{F^{rec}_{tu',tu}} = F^{rec,1}_{tu',tu}, \quad tu', tu \in TU \tag{3.26b}$$

$$F^{in,0}_{tu} + b^\top \alpha_{F^{in}_{tu}} \geq 0, \quad tu \in TU \tag{3.27a}$$
$$A^\top \alpha_{F^{in}_{tu}} = F^{in,1}_{tu}, \quad tu \in TU \tag{3.27b}$$

$$F^{out,0}_{tu} + b^\top \alpha_{F^{out}_{tu}} \geq 0, \quad tu \in TU \tag{3.28a}$$
$$A^\top \alpha_{F^{out}_{tu}} = F^{out,1}_{tu}, \quad tu \in TU \tag{3.28b}$$

$$F^{exit,0}_{tu} + b^\top \alpha_{F^{exit}_{tu}} \geq 0, \quad tu \in TU \tag{3.29a}$$
$$A^\top \alpha_{F^{exit}_{tu}} = F^{exit,1}_{tu}, \quad tu \in TU \tag{3.29b}$$

$$F^{final,0} + b^\top \alpha_{F^{final}} \geq 0 \tag{3.30a}$$
$$A^\top \alpha_{F^{final}} = F^{final,1} \tag{3.30b}$$

$$C^{in,0}_{tu,c} + b^\top \alpha_{C^{in}_{tu,c}} \geq 0, \quad tu \in TU, c \in C \tag{3.31a}$$
$$A^\top \alpha_{C^{in}_{tu,c}} = C^{in,1}_{tu,c}, \quad tu \in TU, c \in C \tag{3.31b}$$

$$C_{tu,c}^{out,0} + b^\top \alpha_{C_{tu,c}^{out}} \geq 0, \quad tu \in TU, c \in C \tag{3.32a}$$
$$A^\top \alpha_{C_{tu,c}^{out}} = C_{tu,c}^{out,1}, \quad tu \in TU, c \in C \tag{3.32b}$$

$$C_c^{final,0} + b^\top \alpha_{C_c^{final}} \geq 0, \quad c \in C \tag{3.33a}$$
$$A^\top \alpha_{C_c^{final}} = C_c^{final,1}, \quad c \in C \tag{3.33b}$$

The linear stochastic LDR model was initially solved using the nominal operating conditions at $\xi^* = 0.5$ obtained by the solving the deterministic NLP model at $\xi^*$, for the range $\xi \in [0.4, 0.6]$. The solver returned model infeasibility errors, and so the range was reduced to $\xi \in [0.45, 0.55]$. The optimal solution for $E[\xi] = 0.5$ was found to be 111.0975 tonne/hr. An example of the resulting optimal network is depicted for $\xi = 0.53$, using the LDR solution for $\xi \in [0.45, 0.55]$ in Figure 3.2. The optimal decision rule parameters for the variables in the model are given in Table 3.2.

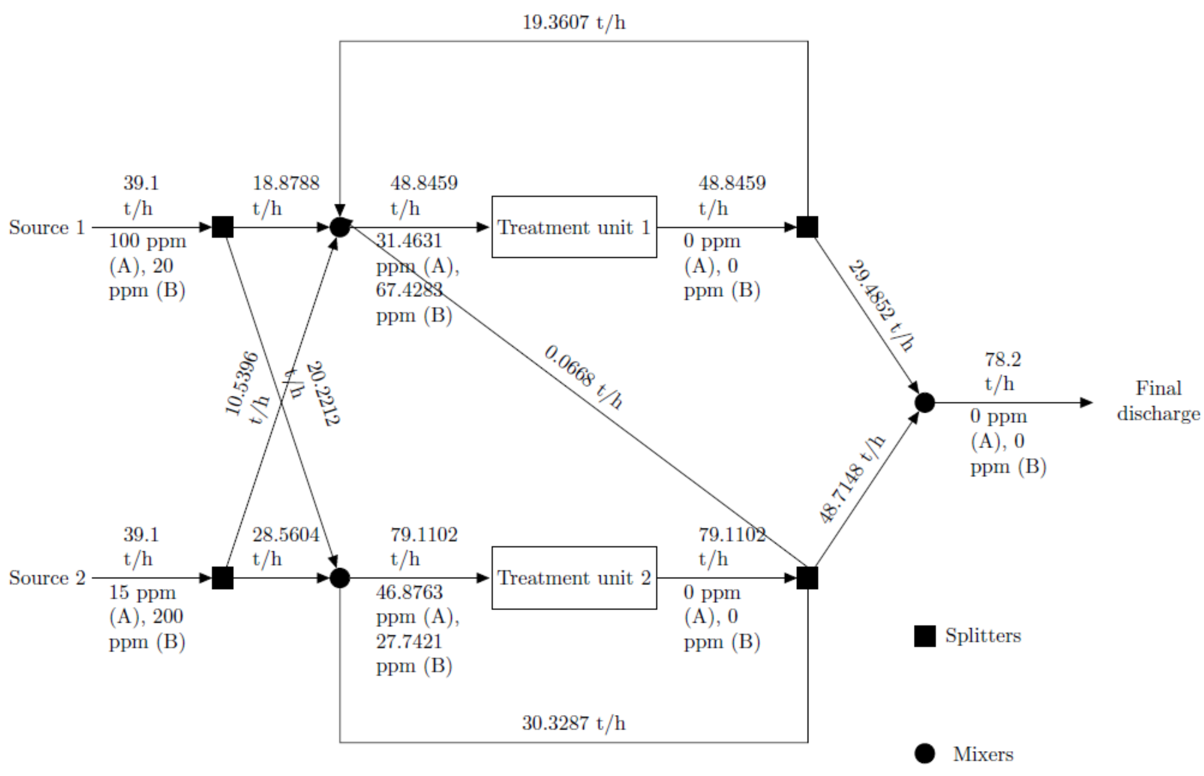


Figure 3.2: Optimal solution for the stochastic LDR formulation of the linearized small water treatment model for $\xi \in [0.45, 0.55]$ at $\xi^* = 0.53$

Table 3.2: Decision rule parameters for the variables in the stochastic LDR formulation of the linearized small water treatment model

| | $\xi \in [0.45, 0.55]$ |
|---|---|
| $F_{s_1,tu_1}$ | 31.3114 - 23.4576$\xi$ |
| $F_{s_1,tu_2}$ | 23.6886 - 6.5424$\xi$ |
| $F_{s_2,tu_1}$ | 10.5396 |
| $F_{s_2,tu_2}$ | 44.4604 - 30$\xi$ |
| $F^{in}_{tu_1}$ | -67.4283 + 219.3854$\xi$ |
| $F^{in}_{tu_2}$ | -102.445 + 342.5664$\xi$ |
| $F^{out}_{tu_1}$ | -67.4283 + 219.3854$\xi$ |
| $F^{out}_{tu_2}$ | -102.445 + 342.5664$\xi$ |
| $F^{rec}_{tu_1,tu_1}$ | -108.9038 + 242.0084$\xi$ |
| $F^{rec}_{tu_2,tu_1}$ | -0.3756 + 0.8346$\xi$ |
| $F^{rec}_{tu_2,tu_2}$ | -170.599 + 379.1088$\xi$ |
| $F^{exit}_{tu_1}$ | 41.4754 - 22.623$\xi$ |
| $F^{exit}_{tu_2}$ | 68.5246 - 37.377$\xi$ |
| $F^{final}$ | 110 - 60$\xi$ |
| $C^{in}_{tu_1,A}$ | 337.1417 - 576.7521$\xi$ |
| $C^{in}_{tu_1,B}$ | 67.4283 |
| $C^{in}_{tu_2,A}$ | 53.5574 - 12.6059$\xi$ |
| $C^{in}_{tu_2,B}$ | 676.2301 - 1223.5622$\xi$ |
| $C^{out}_{tu_1,A}$ | 0 |
| $C^{out}_{tu_1,B}$ | 0 |
| $C^{out}_{tu_2,A}$ | 0 |
| $C^{out}_{tu_2,B}$ | 0 |
| $C^{final}_{A}$ | 0 |
| $C^{final}_{B}$ | 0 |

It was observed that the solution satisfied all flow balance equations in the model. However, neither the solution to the linearized LP formulation nor to the stochastic LDR model satisfied the original component balances in the model. It was inferred that the violation of component balances occurred as a consequence of inadequate linearization, and solving the model to satisfy these modified equations. Therefore, the linearized solution was deemed infeasible due to component balance violations throughout the model. This infeasibility was found to propagate into the stochastic LDR model as well, and hence, the optimal decision rules obtained from the stochastic LDR model were deemed infeasible.

## 3.4 Concluding remarks

This chapter presented the application of the affine decision rule-based stochastic optimization method on the linearized formulation of the small water treatment model. The usage of first order Taylor series approximation for the linearization of a nonlinear model around its nominal conditions was discussed in Section 3.1, and its application on the small water treatment model was depicted in Section 3.2. The stochastic LDR-based formulation of the linearized model under uncertainty was depicted in Section 3.3. It was observed that, due to inadequate linearization of the NLP model around nominal conditions, the decision rules obtained for the model variables lead to violation of the component balance constraints, thereby rendering the decision rules/policies infeasible for practical application. Furthermore, it was observed that the stochastic LDR model itself was only feasible for a very small range of $\xi$. It can, therefore, be inferred that, even if the model was modified such that flow and component balance violations were no longer violated, linearization around multiple conditions might be necessary to obtain decision rules for the entire range of uncertainty defined.

# Chapter 4

# Nonlinear Robust Optimization using the Affine Decision Rule

In this chapter, the application of the nonlinear robust optimization technique, using the affine decision rule, developed by Yuan, et al. [46], was evaluated on the small water treatment model. Chapters 2 and 3 present the solution to the stochastic LDR formulation of the small water treatment model linearized using McCormick relaxation, and first order Taylor series approximation, respectively. These approaches were sequential in nature - first, the relaxed LP/linearized model were formulated; then, the stochastic LDR-based models were developed. The method explored in this chapter follows a different solution procedure, in which the affine adjustable robust counterpart has been directly derived for a general MINLP model. This method is discussed in Section 4.1, and the derived nonlinear robust counterpart of the model is presented in Section 4.2. The improved solution to the model is also discussed in the same section.

## 4.1 Nonlinear robust process optimization framework

Yuan, et al. (2018) [46] proposed a novel nonlinear robust optimization framework to tackle nonlinear process design problems containing uncertain parameters. This framework involves linearization of the model with respect to uncertainty, around multiple realizations of the same, and presents an iterative algorithm to tackle the problem.

First, the general optimization problem under uncertainty is classified into three categories. In problems belonging to the first category, the uncertain parameters are only

assumed to be involved in the inequality constraints of the model. Typically, process design problems that contain only static decisions belong to this category. For such problems, no equality constraints exist, and so, the robust counterpart to the inequality constraints are obtained by directly applying the approach detailed in Section 1.6.4 [45], on the linearized constraints. For the second category of problems, the model is assumed to contain both static design, as well as state variables linked by a set of equality and inequality constraints. Due to the presence of equality constraints in the model, the robust counterpart is not directly derived; rather, the design variables are assumed to be first-stage/fixed decisions, while the state variables are assumed to be second-stage/recourse variables. The state variables are substituted by functions of uncertainty and design variables, applying the Implicit Function Theorem to the equality constraints. The robust counterpart to the inequality constraints is obtained in a similar manner to problems of the first category. The third category of problems covers the general optimization problem containing design, state, as well as control variables. In such problems, the design variables are assumed to be fixed decisions taken before uncertainty is realized; however, both state and control variables are assumed to be dependent on the realization of uncertainty. Furthermore, the control variables are assumed to be affinely adjustable to uncertainty, and this assumption is reflected in the reformulation of the control variables in the model using the affine decision rule (LDR). Applying the LDR formulation to the control variables reduces the nature of the problem to the second category, and the adjustable robust counterpart to the original nonlinear problem is obtained.
The general optimization problem is given as:

$$\begin{aligned}
&\min_{u,y(\xi),z(\xi)} \quad \phi(u,y,z) \\
&\text{subject to} \\
&F(\xi,u,y(\xi),z(\xi)) = 0 \\
&G(\xi,u,y(\xi),z(\xi)) \leq 0
\end{aligned}$$

Using the developed nonlinear robust optimization approach, the control variables $z(\xi)$, present in both equality and inequality constraints, are first reformulated as follows.

$$z(\xi) = z^0 + z^1\xi$$

Each equality constraint (contained in $F(\xi, u, y(\xi), z(\xi))$) is robustly reformulated using implicit derivatives of the equality function with respect to uncertainty, state variables and control variables, denoted by $F_\xi$, $F_y$ and $F_z$ respectively, as well as derivatives of the state and control variables with respect to $\xi$, given as $y_\xi$ and $z^1$, respectively. Each inequality constraint (contained in $G(\xi, u, y(\xi), z(\xi))$) is initially linearized using first order Taylor series approximation around a specific realization of uncertainty ($\xi$). The resulting linearized inequality constraint, containing a first-order partial derivative of the inequality function with respect to $\xi$, denoted by $\nabla_\xi G(\xi, u, y(\xi), z(\xi))$, is robustly reformulated. All derivatives involved in this robust counterpart are evaluated at $\xi^*$.

The robust counterpart of this nonlinear optimization problem is thus given as follows. In the following model, the inequality constraint is still semi-infinite in nature, and therefore, its robust counterpart must be derived using duality.

$$\min_{u,y(\xi),z(\xi)} \quad \phi(u, y, z)$$

subject to

$$F(\xi^*, u, y(\xi^*), z(\xi^*)) = 0$$

$$F_y y_\xi + F_z z^1 + F_\xi = 0$$

$$[G(\xi^*, u, y(\xi^*), z(\xi^*)) - \xi^* \nabla_\xi G(\xi^*, u, y(\xi^*), z(\xi^*))] + \xi[\nabla_\xi G(\xi^*, u, y(\xi^*), z(\xi^*))] \leq 0$$

**Illustrative example**

The derivation of the affine adjustable robust counterpart of the general optimization problem containing design, state, and control variables is illustrated in the following example.

$$\min_{u,y(\xi),z(\xi)} \quad \phi(u, y, z)$$

subject to

$$a_1 y_1(\xi) + a_2 y_2(\xi) + c z(\xi) = 0$$

$$y_1(\xi) + z(\xi) \leq u y_2(\xi)$$

Applying the affine decision rule formulation to $z(\xi)$, the problem is redefined as follows.

$$\begin{aligned}
&\min_{u, y_1(\xi), y_2(\xi), z(\xi)} \quad \phi(u, y, z) \\
&\text{subject to} \\
&a_1 y_1(\xi) + a_2 y_2(\xi) + c(z^0 + z^1 \xi) = 0 \\
&y_1(\xi) + (z^0 + z^1 \xi) - u y_2(\xi) \leq 0
\end{aligned}$$

The equality constraints are reformulated using the following derivatives,

$$F_{y_1} = a_1, \qquad F_{y_2} = a_2, \qquad F_z = c$$

to give,

$$\begin{aligned}
&a_1 y_1(\xi^*) + a_2 y_2(\xi^*) + c(z^0 + z^1 \xi^*) = 0 \\
&a_1 y_{1_\xi} + a_2 y_{2_\xi} + c z^1 = 0
\end{aligned}$$

The inequality constraints are linearized with respect to uncertainty, as follows,

$$y_1(\xi^*) + (z^0 + z^1 \xi^*) - u y_2(\xi^*) + (\xi - \xi^*) \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \leq 0, \quad \forall \xi \in \Xi$$

$$\begin{aligned}
y_1(\xi^*) + (z^0 + z^1 \xi^*) - u y_2(\xi^*) - \xi^* \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \\
+ \xi \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \leq 0, \quad \forall \xi \in \Xi
\end{aligned}$$

Using the technique described in Section 1.6.4,

$$\begin{aligned}
- y_1(\xi^*) - (z^0 + z^1 \xi^*) + u y_2(\xi^*) + \xi^* \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \\
+ \begin{bmatrix} \min_{\xi} \quad \xi \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \\ \text{subject to} \\ \boldsymbol{A} \xi \geq \boldsymbol{b} \end{bmatrix} \geq 0
\end{aligned}$$

$$\begin{aligned}
- y_1(\xi^*) - (z^0 + z^1 \xi^*) + u y_2(\xi^*) + \xi^* \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \\
+ \begin{bmatrix} \max_{\boldsymbol{\lambda} \geq 0} \quad (\boldsymbol{b}^\top \boldsymbol{\lambda}) \\ \text{subject to} \\ \boldsymbol{A}^\top \boldsymbol{\lambda} = \nabla_\xi y_1(\xi) + z(\xi) - u y_2(\xi) \Big|_{\xi^*} \end{bmatrix} \geq 0
\end{aligned}$$

to give,

$$-y_1(\xi^*) - (z^0 + z^1\xi^*) + uy_2(\xi^*) + \xi^*\nabla_\xi y_1(\xi) + z(\xi) - uy_2(\xi)\Big|_{\xi^*} + b^\top \boldsymbol{\lambda} \geq 0$$

$$A^\top \boldsymbol{\lambda} = \nabla_\xi y_1(\xi) + z(\xi) - uy_2(\xi)\Big|_{\xi^*}$$

The final robust counterpart to this illustrative nonlinear problem is, thus, given as,

$$\min_{u,y(\xi),z(\xi)} \phi(u,y,z)$$

subject to

$$a_1y_1(\xi^*) + a_2y_2(\xi^*) + c(z^0 + z^1\xi^*) = 0$$

$$a_1y_{1_\xi} + a_2y_{2_\xi} + cz^1 = 0$$

$$-y_1(\xi^*) - (z^0 + z^1\xi^*) + uy_2(\xi^*) + \xi^*\nabla_\xi y_1(\xi) + z(\xi) - uy_2(\xi)\Big|_{\xi^*} + b^\top \boldsymbol{\lambda} \geq 0$$

$$A^\top \boldsymbol{\lambda} = \nabla_\xi y_1(\xi) + z(\xi) - uy_2(\xi)\Big|_{\xi^*}$$

$$\boldsymbol{\lambda} \geq 0$$

The authors [46] contrasted the original nonlinear model with the robust counterpart with respect to problem size, and made the following observations. The number of equality constraints increases two-fold since a single equality constraint is robustly reformulated into two constraints, and the robust counterpart to original inequality constraints involves a new equality constraint. This also leads to an increase in the number of variables due to the present of implicit derivatives, as well as first order derivative terms for the original inequalities. The number of inequalities remains the same in the robust counterpart, as in the original model. However, new dual variables ($\lambda$) of the size of $\boldsymbol{b}$ are introduced in the stochastic LDR model, for every inequality constraint. Therefore, the robust counterpart of the stochastic LDR model always contains a larger set of constraints, as well as variables, than the original model. The significant increase in the size of the variables set is not quite evident in the case of the small water treatment model; however, this increase is very apparent in the case of the SAGD model, explored further in Chapter 5.

## 4.2 Robust counterpart of nonlinear LDR-based formulation of the small water treatment model

The uncertainty in model (Section 2.2) was sourced from source flow ($F_s(\xi)$) and as a result, all the state and control variables in the model were assumed to be dependent on uncertainty. In this problem, the source flow $F_s$ was assumed to be the uncertain parameter, depending on primitive uncertainty $\xi$, as follows,

$$F_s(\xi) = \xi F_s^1 + (1 - \xi)F_s^2, \quad \forall s \in S$$

where $F_s^1$ and $F_s^2$ were taken to be the extreme points for the realizations of $F_s$. The source flow was assumed to vary between 25 tonne/hr ($F_s^1$) and 55 tonne/hr ($F_s^2$).

The variables present in the model were classified into state and control variables and presented in Table 4.1. The control variables were reformulated using the affine decision rule, as follows:

$$\begin{aligned}
F_{s,tu}(\xi) &= F_{s,tu}^0 + F_{s,tu}^1\xi, \quad \forall s \in S, tu \in TU, \xi \in \Xi \\
F_{tu,tu'}^{rec}(\xi) &= F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1}\xi, \quad \forall tu, tu' \in TU, \xi \in \Xi \\
F_{tu}^{exit}(\xi) &= F_{tu}^{exit,0} + F_{tu}^{exit,1}\xi, \quad \forall tu \in TU, \xi \in \Xi
\end{aligned}$$

Table 4.1: Classification of state and control variables in the small water treatment model

| State variables $y(\xi)$ | Control variables $z(\xi)$ |
|---|---|
| $F_{tu}^{in}$ | $F_{s,tu}$ |
| $F_{tu}^{out}$ | $F_{tu}^{exit}$ |
| $C_{tu,c}^{in}$ | $F_{tu',tu}^{rec}$ |
| $C_{tu,c}^{out}$ | |
| $F^{final}$ | |
| $C_c^{final}$ | |

The stochastic LDR model linearized around $\xi^* = 0.5$ was developed using the deterministic formulation of the model in Section 2.2. The implicit derivatives of the state variables ($m(\xi)$) are denoted by $y_m$. The dual variables associated with the robust counterparts of the concentration limits and non-negativity constraints are denoted by $\alpha_g$, where $g$ represents the inequality constraint that the dual is derived for, and $\lambda$, respectively. The decision rule parameters for the control variables that are optimized by this model are grouped into $F^0$ and $F^1$. The same set of design variables, as in the deterministic formulation, are optimized by the nonlinear robust model, in addition to the state variables.

$$\min \sum_{tu} F_{tu}^{in}(\xi^*) \tag{4.1}$$

subject to

$$F_s^2 + \xi^*(F_s^1 - F_s^2) - \left(\sum_{tu} F_{s,tu}^0 + F_{s,tu}^1 \xi^*\right) = 0, \quad \forall s \in S \tag{4.2a}$$

$$(F_s^1 - F_s^2) - \left(\sum_{tu} F_{s,tu}^1\right) = 0, \quad \forall s \in S \tag{4.2b}$$

$$\left(\sum_{s} F_{s,tu}^0 + F_{s,tu}^1 \xi^*\right) + \left(\sum_{tu'} F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1} \xi^*\right) - F_{tu}^{in}(\xi^*) = 0, \quad \forall tu \in TU \tag{4.3a}$$

$$\left(\sum_{s} F_{s,tu}^1\right) + \left(\sum_{tu'} F_{tu',tu}^{rec,1}\right) - y_{F_{tu}^{in}} = 0, \quad \forall tu \in TU \tag{4.3b}$$

$$F_{tu}^{in}(\xi^*) - F_{tu}^{out}(\xi^*) = 0, \quad tu \in TU \tag{4.4a}$$

$$y_{F_{tu}^{in}} - y_{F_{tu}^{out}} = 0, \quad \forall tu \in TU \tag{4.4b}$$

$$F_{tu}^{out}(\xi^*) - \left(\sum_{tu'} F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1} \xi^*\right) - (F_{tu}^{exit,0} + F_{tu}^{exit,1} \xi^*) = 0, \quad \forall tu \in TU \tag{4.5a}$$

$$y_{F_{tu}^{out}} - \left(\sum_{tu'} F_{tu,tu'}^{rec,1}\right) - F_{tu}^{exit,1} = 0, \quad \forall tu \in TU \tag{4.5b}$$

$$\left(\sum_{tu} F_{tu}^{exit,0} + F_{tu}^{exit,1} \xi^*\right) - F^{final}(\xi^*) = 0 \tag{4.6a}$$

$$\left(\sum_{tu} F_{tu}^{exit,1}\right) - y_{F^{final}} = 0 \tag{4.6b}$$

$$\left(\sum_{s} (F_{s,tu}^0 + F_{s,tu}^1 \xi^*) C_{s,c}\right) + \left(\sum_{tu'} (F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1} \xi^*) C_{tu',c}^{out}(\xi^*)\right)$$
$$- F_{tu}^{in}(\xi^*) C_{tu,c}^{in}(\xi^*) = 0, \quad \forall tu \in TU, c \in C \tag{4.7a}$$

$$\left(\sum_{s} F_{s,tu}^1 C_{s,c}\right) + \left(\sum_{tu'} C_{tu',c}^{out}(\xi^*) F_{tu',tu}^{rec,1} + (F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1} \xi^*) y_{C_{tu',c}^{out}}\right)$$
$$- (C_{tu,c}^{in}(\xi^*) y_{F_{tu}^{in}} + F_{tu}^{in}(\xi^*) y_{C_{tu,c}^{in}}) = 0, \quad \forall tu \in TU, c \in C \tag{4.7b}$$

$$F^{in}_{tu}(\xi^*)C^{in}_{tu,c}(\xi^*)[1 - RR_{tu,c}] - F^{out}_{tu}(\xi^*)C^{out}_{tu,c}(\xi^*) = 0, \quad \forall tu \in TU, c \in C \tag{4.8a}$$

$$\begin{aligned}[1 - RR_{tu,c}](C^{in}_{tu,c}(\xi^*)y_{F^{in}_{tu}} + F^{in}_{tu}(\xi^*)y_{C^{in}_{tu,c}}) \\ - (C^{out}_{tu,c}(\xi^*)y_{F^{out}_{tu}} + F^{out}_{tu}(\xi^*)y_{C^{out}_{tu,c}}) = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{4.8b}$$

$$\begin{aligned}F^{out}_{tu}(\xi^*)C^{out}_{tu,c}(\xi^*) - \left(\sum_{tu'}(F^{rec,0}_{tu,tu'} + F^{rec,1}_{tu,tu'}\xi^*)C^{out}_{tu,c}(\xi^*)\right) \\ - (F^{exit,0}_{tu} + F^{exit,1}_{tu}\xi^*)C^{out}_{tu,c}(\xi^*) = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{4.9a}$$

$$\begin{aligned}(C^{out}_{tu,c}(\xi^*)y_{F^{out}_{tu}} + F^{out}_{tu}(\xi^*)y_{C^{out}_{tu,c}}) - \left(\sum_{tu'} C^{out}_{tu,c}(\xi^*)F^{rec,1}_{tu,tu'} + (F^{rec,0}_{tu,tu'} + F^{rec,1}_{tu,tu'}\xi^*)y_{C^{out}_{tu,c}}\right) \\ - (C^{out}_{tu,c}(\xi^*)F^{exit,1}_{tu}) - (F^{exit,0}_{tu} + F^{exit,1}_{tu}\xi^*)y_{C^{out}_{tu,c}} = 0, \quad \forall tu \in TU, c \in C\end{aligned} \tag{4.9b}$$

$$\left(\sum_{tu}(F^{exit,0}_{tu} + F^{exit,1}_{tu}\xi^*)C^{out}_{tu,c}(\xi^*)\right) - (F^{final}(\xi^*)C^{final}_{c}(\xi^*)) = 0, \quad \forall c \in C \tag{4.10a}$$

$$\begin{aligned}\left(\sum_{tu} C^{out}_{tu,c}(\xi^*)F^{exit,1}_{tu}\right) + \left(\sum_{tu}(F^{exit,0}_{tu} + F^{exit,1}_{tu}\xi^*)y_{C^{out}_{tu,c}}\right) \\ - (C^{final}_{c}(\xi^*)y_{F^{final}} + F^{final}(\xi^*)y_{C^{final}_{c}}) = 0, \quad \forall c \in C\end{aligned} \tag{4.10b}$$

$$\xi^*\nabla_{C^{final}_c} - (C^{final}_c(\xi^*) - C^{target}_c) + b^\top\lambda_c \geq 0 \tag{4.11a}$$

$$A^\top\lambda_c + \nabla_{C^{final}_c} = 0 \tag{4.11b}$$

$$\lambda_c \geq 0 \tag{4.11c}$$

$$F^0_{s,tu} + b^\top\alpha_{F_{s,tu}} \geq 0, \quad s \in S, tu \in TU \tag{4.12a}$$

$$A^\top\alpha_{F_{s,tu}} = F^1_{s,tu}, \quad s \in S, tu \in TU \tag{4.12b}$$

$$F^{rec,0}_{tu,tu'} + b^\top\alpha_{F^{rec}_{tu,tu'}} \geq 0, \quad tu, tu' \in TU \tag{4.13a}$$

$$A^\top\alpha_{F^{rec}_{tu,tu'}} = F^{rec,1}_{tu,tu'}, \quad tu, tu' \in TU \tag{4.13b}$$

$$F^{exit,0}_{tu} + b^\top\alpha_{F^{exit}_{tu}} \geq 0, \quad tu \in TU \tag{4.14a}$$

$$A^\top\alpha_{F^{exit}_{tu}} = F^{exit,1}_{tu}, \quad tu \in TU \tag{4.14b}$$

The nonlinear robust LDR model was derived around the nominal condition, i.e., $\xi^* = 0.5$, where the objective function was minimized for $\xi^*$. The model was derived for different ranges of uncertainty, $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$. The model was solved in GAMS using the ANTIGONE NLP solver, using a pre-solving step with the

IPOPT NLP solver, to facilitate a quicker solution. The locally optimal objective at $\xi^* = 0.5$ was found to be 89.8361 for both $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$. An example for the resulting network flows is depicted for $\xi = 0.53$, using the LDR solutions for $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$, in Figures 4.1 and 4.2 respectively. The evolution of the optimal objective and computed concentration profiles for $C_c^{final}$ for both ranges of uncertainty are shown in Figure 4.3. The optimal decision rule parameters for the control variables in the model are given in Table 4.2.

Table 4.2: Decision rule parameters for the control variables in the nonlinear robust LDR formulation of the small water treatment model

| | $\xi \in [0.4, 0.6]$ | $\xi \in [0, 1]$ |
|---|---|---|
| $F_{s_1,tu_1}$ | 55 - 30$\xi$ | 55 - 30$\xi$ |
| $F_{s_2,tu_2}$ | 55 - 30$\xi$ | 55 - 30$\xi$ |
| $F^{rec}_{tu_1,tu_2}$ | 14.3621 - 9.0521$\xi$ | 9.9226 - 0.1731$\xi$ |
| $F^{exit}_{tu_1}$ | 40.6379 - 20.9479$\xi$ | 45.0774 - 29.8269$\xi$ |
| $F^{exit}_{tu_2}$ | 69.3621 - 39.0521$\xi$ | 64.9226 - 30.1731$\xi$ |

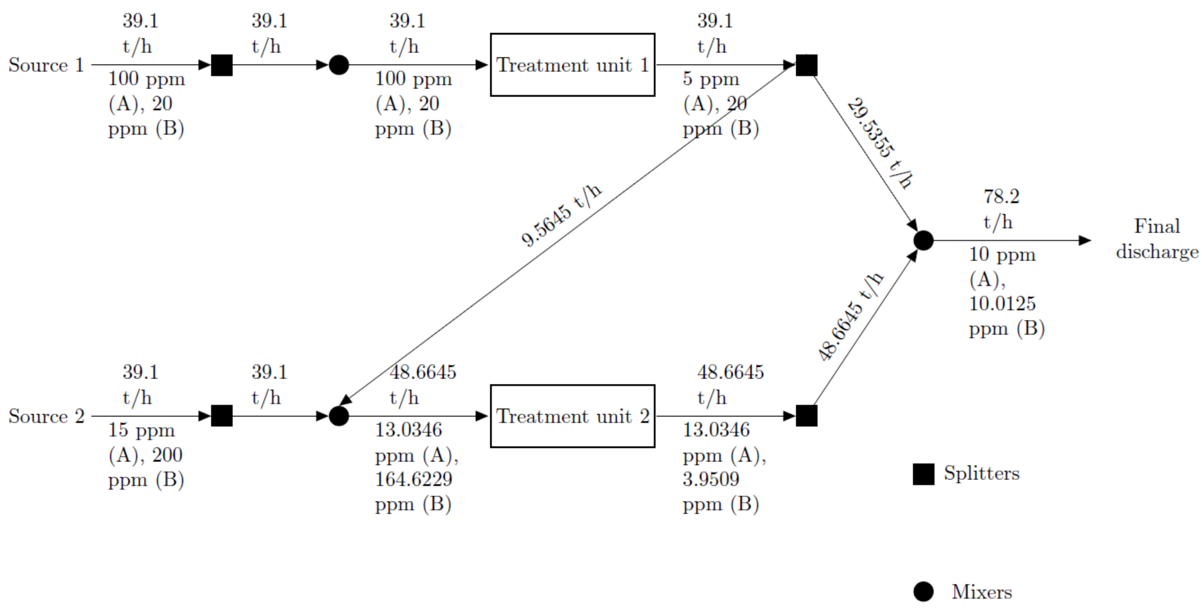


Figure 4.1: Optimal solution for the nonlinear robust LDR formulation of the small water treatment model for $\xi \in [0.4, 0.6]$ at $\xi^* = 0.53$

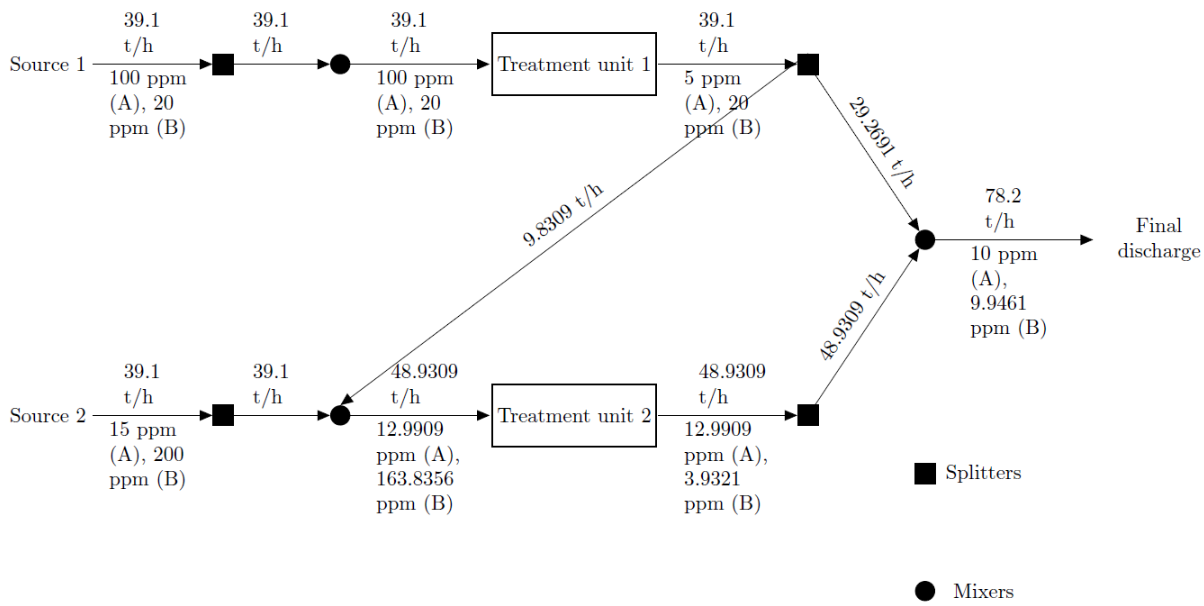


Figure 4.2: Optimal solution for the nonlinear robust LDR formulation of the small water treatment model for $\xi \in [0, 1]$ at $\xi^* = 0.53$

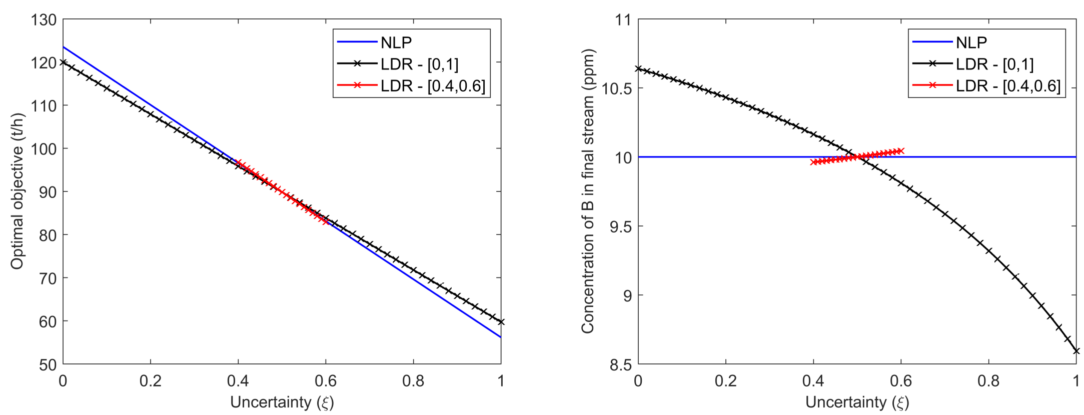


Figure 4.3: Evolution of optimal objective using LDR models (left), and computed concentration profile for contaminant $B$ (right)

The first observation made using the decision rules for both ranges of uncertainty was that the solution was feasible with respect to flow rate and component balances. However, it was also observed that when the nonlinear robust LDR model was solved for either range of uncertainty, the computed concentration profiles for $C_B^{final}$ violated the target (10 ppm). The profiles were also observed to be monotonically decreasing in nature. The cause for violation of the target was inferred to be the approximated nature of the linearized model. The model was re-solved for a stricter target of 9.5

ppm on $C_B^{target}$, and the solution was found to be robustly feasible with no target violation. However, this heuristic method of re-solving the model for stricter targets was found to lead to overly conservative solutions. To deal with this issue, an alternative scheme was proposed. The original NLP target concentration inequality constraints (Equation 2.11) (and as a result, the balance equations 2.2 - 2.10) were enforced at the terminal points of the uncertainty set ($\xi^{low}$ and $\xi^{high}$) considered in the model. The modified model is given as follows.

min [Equation 4.1]

subject to

[Equations 4.2a - 4.14b]

$$XF_s^1 + (1-X)F_s^2 = \sum_{tu} F_{s,tu}^0 + F_{s,tu}^1 X, \quad \forall s \in S, X \in \{\xi^{low}, \xi^{high}\} \tag{4.15}$$

$$\sum_{tu} F_{s,tu}^0 + F_{s,tu}^1 X + \sum_{tu'} F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1} X = F_{tu,X}^{in}, \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \tag{4.16}$$

$$F_{tu,X}^{in} = F_{tu,X}^{out}, \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \tag{4.17}$$

$$\begin{aligned} F_{tu,X}^{out} = &\left( \sum_{tu'} F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1} X \right) \\ &+ \left( F_{tu}^{exit,0} + F_{tu}^{exit,1} X \right), \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \end{aligned} \tag{4.18}$$

$$\left( \sum_{tu} F_{tu}^{exit,0} + F_{tu}^{exit,1} X \right) = F_X^{final}, X \in \{\xi^{low}, \xi^{high}\} \tag{4.19}$$

$$\begin{aligned} &\sum_{s} (F_{s,tu}^0 + F_{s,tu}^1 X) C_{s,c} + \sum_{tu'} (F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1} X) C_{tu',c,X}^{out} \\ &= C_{tu,c,X}^{in} F_{tu,X}^{in}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \end{aligned} \tag{4.20}$$

$$\begin{aligned} &C_{tu,c,X}^{in} F_{tu,X}^{in} = C_{tu,c,X}^{out} F_{tu,X}^{out} + C_{tu,c,X}^{in} F_{tu,X}^{in} RR_{tu,c}, \\ &\forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \end{aligned} \tag{4.21}$$

$$\begin{aligned} F_{tu,X}^{out} C_{tu,c,X}^{out} = &\sum_{tu'} (F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1} X) C_{tu,c,X}^{out} \\ &+ (F_{tu}^{exit,0} + F_{tu}^{exit,1} X) C_{tu,c,X}^{out}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \end{aligned} \tag{4.22}$$

$$\sum_{tu} (F_{tu}^{exit,0} + F_{tu}^{exit,1} X) C_{tu,c}^{\text{out}} = C_{c,X}^{\text{final}} F_X^{\text{final}}, \quad \forall c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{4.23}$$

$$C^{\text{final}}_{c,X} \leq C^{\text{target}}_{c}, \quad \forall c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{4.24}$$

Solving this modified model gave a robustly feasible solution with an optimal objective value of 99.9107 tonne/hr at $\xi^* = 0.5$, for both $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$. It was observed that the solution to the modified model provided a feasible solution for the entire range of uncertainty, with no target violations, nor violation of flow and component balances. An example for the resulting network is depicted for $\xi = 0.53$, using the LDR solution for $\xi \in [0.4, 0.6]$ in Figure 4.4. The evolution of the optimal objective, and the computed concentration profiles for $C_B^{final}$ for both ranges of uncertainty are shown in Figure 4.5. The optimal decision rule parameters for the control variable in the modified LDR model are given in Table 4.3.

Table 4.3: Decision rule parameters for the control variables in the modified nonlinear robust LDR formulation of the small water treatment model

| | $\xi \in [0.4, 0.6]$ | $\xi \in [0, 1]$ |
|---|---|---|
| $F_{s_1,tu_1}$ | 52.8871 - 28.8475$\xi$ | 52.8871 - 28.8475$\xi$ |
| $F_{s_1,tu_2}$ | 2.1129 - 1.1525$\xi$ | 2.1129 - 1.1525$\xi$ |
| $F_{s_2,tu_2}$ | 55 - 30$\xi$ | 55 - 30$\xi$ |
| $F^{rec}_{tu_1,tu_2}$ | 13.6886 - 7.4665$\xi$ | 13.6886 - 7.4665$\xi$ |
| $F^{rec}_{tu_2,tu_1}$ | 13.6886 - 7.4665$\xi$ | 13.6886 - 7.4665$\xi$ |
| $F^{exit}_{tu_1}$ | 52.8871 - 28.8475$\xi$ | 52.8871 - 28.8475$\xi$ |
| $F^{exit}_{tu_2}$ | 57.1129 - 31.1525$\xi$ | 57.1129 - 31.1525$\xi$ |

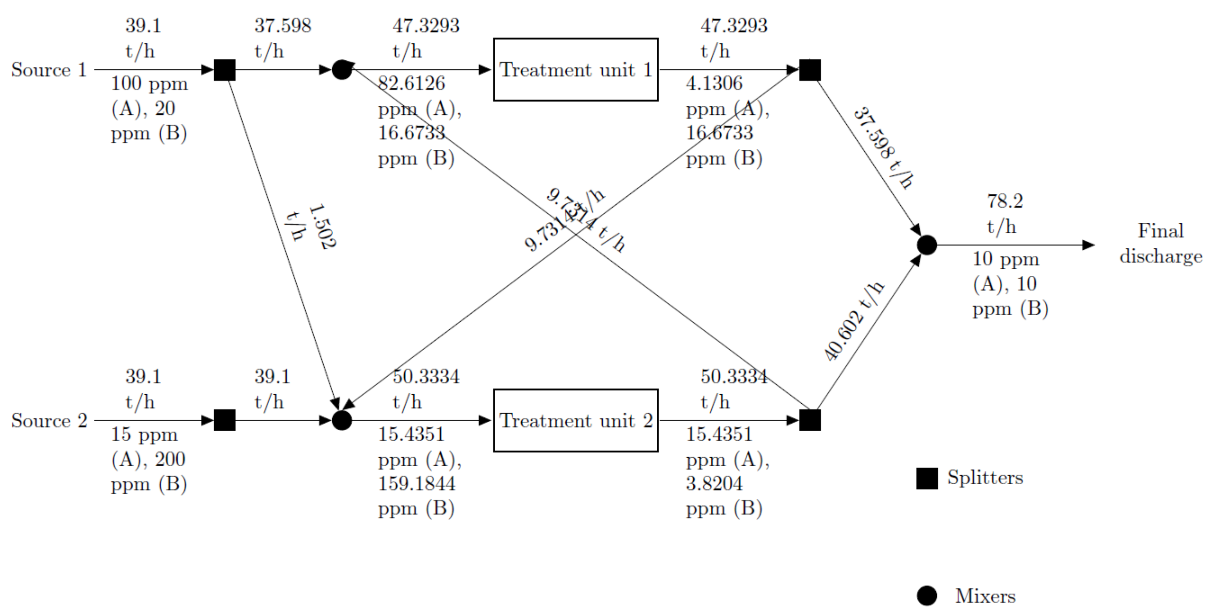


Figure 4.4: Optimal solution for the modified nonlinear robust LDR formulation of the small water treatment model for $\xi \in [0.4, 0.6]$ at $\xi^* = 0.53$

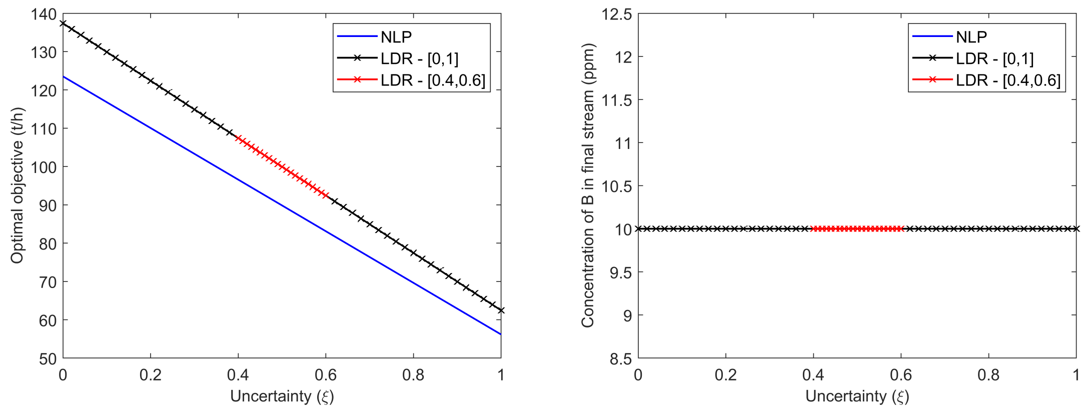


Figure 4.5: Evolution of optimal objective using modified LDR models (left), and computed concentration profile for contaminant $B$ (right)

## 4.3 Concluding remarks

This chapter presented the application of the two-stage nonlinear robust optimization technique developed by Yuan, et al. [46] on the small water treatment model. The nonlinear robust optimization technique was detailed and illustrated in Section 4.1, and its application on the small water treatment model was depicted in Section 4.2. The defining feature of this technique compared to the techniques used in Chapters 2 and 3, was that the decision rules obtained for the control variables did not lead to the violation of the component balance constraints. However, using these decision rules, violations of the final target concentration were observed, and so, an alternative scheme was proposed to tackle this violation. Using the solution from the modified robust LDR model, it was observed that the decision rules successfully provided feasible solutions with respect to both target concentrations, as well flow and component balances, for the entire range of uncertainty.

# Chapter 5

# Nonlinear Robust Optimization of the SAGD Effluent Treatment System

In this chapter, the application of the nonlinear robust optimization technique, using the affine decision rule, developed by Yuan, et al. [46], was evaluated on the SAGD effluent treatment and steam generation network. Section 5.1 provides background on SAGD operations, and Section 5.2 presents the deterministic formulation of the SAGD model, and discusses its optimal solution. The derivation and solution of the nonlinear robust counterpart of the SAGD model under steam demand uncertainty is presented in Section 5.3. The proposed model reformulation, and algorithm for an improved solution are discussed in Section 5.4, and the results for the same are discussed in Section 5.5.

## 5.1 Overview of SAGD operations

The Steam Assisted Gravity Drainage (SAGD) process [47] is a method of oil recovery that is used for production of bitumen and heavy crude oils [48]. In this process, pairs of horizontal wells are drilled into the oil reservoir. The top well is known as the injection well, while the bottom well is termed as the production well. Steam generated at the surface is directed into the injection well, and serves to heat the oil and lower its viscosity. The bitumen or crude oil, now with reduced viscosity, is produced from the bottom well. The production output from this process is an emulsion of oil, water, sand and clay. This emulsion is passed to the central processing facility and goes through the stages of oil/water separation, effluent treatment, and steam generation. The overall superstructure for the SAGD effluent treatment and steam generation system, with all possible flow streams, is depicted in Figure 5.1.

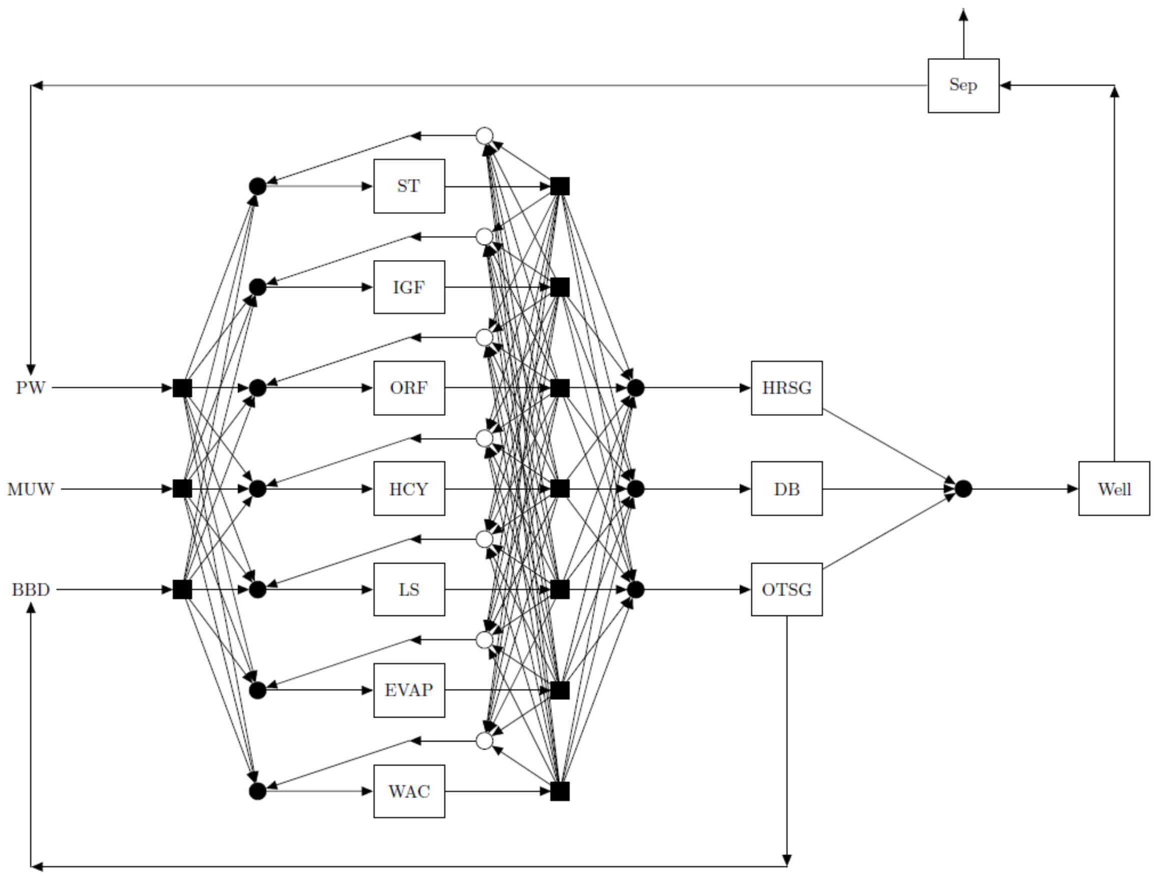


Figure 5.1: Superstructure of the SAGD effluent treatment and steam generation network

The main objective of the effluent treatment process in SAGD operations is to treat the produced water ($PW$) from the bitumen emulsion to meet the boiler feed requirements, while generating steam to meet the demand from the reservoir. The process is, therefore, to be optimized such that water is recycled as much as possible in the process, and to cut down on the makeup water requirements. The main target in the process is the boiler feed water concentration level for each contaminant; however, there are limits imposed on inlet contaminant concentration to each treatment unit in the process. Therefore, the aim of optimization of this model is to obtain an optimal network design, feasible for all realizations of uncertainty in the chosen range, with respect to target concentration limits under cost optimization.

The SAGD model used in this chapter considers three streams, grouped into set $S$ - produced water ($PW$), makeup water ($MUW$), and boiler blowdown ($BBD$). The major contaminants found in the produced water stream are oil ($O$), silica ($Si$), metal ions measured in terms of total hardness ($TH$), and total suspended solids ($TSS$). The variables used in the model are given in Table 5.1. The general concentration of these contaminants in all three water streams is given in Table 5.2 [2]. Several treatment options are available to handle the task of treating these streams as per the specified targets; seven such treatment units, grouped into set $TU$, are chosen in this superstructure - skim tank ($ST$), induced gas flotation unit ($IGF$), oil removal filter ($ORF$), hydrocyclone ($HCY$), lime softening unit ($LS$), evaporator ($EVAP$), and weak acid cation exchanger ($WAC$). The contaminant removal efficiencies for each treatment unit are listed in Table 5.3 [2].

The treated streams are passed into one or more steam generation units, grouped into set $SGU$ - heat recovery steam generator ($HRSG$), drum boiler ($DB$), and once-through steam generator ($OTSG$). Once-through steam generators typically produce 75-80% quality steam; the water that is left over from steam generation in this unit is supplied back to the treatment process as the boiler blowdown stream [2]. Drum boilers produce nearly 100% quality steam, whereas heat-recovery steam generation units can be used as internal power sources in the model; the use of these units comes at the expense of higher capital costs and electricity usage. The steam generated is passed into the injection well ($WI$) at the reservoir. It is worthwhile to mention that although in this thesis the objective is to minimize total cost of treatment as a function of flow rates, an optimization model solving for both flow-rate and energy consumption minimization can be solved. In this chapter, the source flow variable cost, as well as fixed and variable costs associated with each treatment unit in $TU$ are assumed to be affine functions of stream flow ($F_s$) and treatment unit inflow ($F_{tu}^{in}$) rates, respectively.

## 5.2 Deterministic formulation

The SAGD model is described as a set of mass flow, and component concentration balances over all the units in the model, as well as upper and lower limits on all flow rates, in addition to auxiliary constraints. Equations 5.2 - 5.2 and 5.18 - 5.26 describe the flow rate balances and limits, respectively. The component balances and limits are specified by Equations 5.2 - 5.2 and 5.2 - 5.2, respectively. The remaining equations in the model enforce additional constraints and logical connections, and compute costs involved in the model. The sets of variables optimized in this model are given in Table 5.1. The input and operational parameters in the model are given in Tables 5.2 and 5.3. The cost function parameters are listed in Tables 5.4 and 5.5. The maximum allowable inlet concentration to the treatment units ($C^{max}_{tu,c}$), target inlet concentrations to the steam generation units ($C^{target}_{sgu,c}$), and other parameters used in the model are listed in Table 5.6 [2].

$$\min \quad \left(\sum_{s} cost_s\right) + \left(\sum_{tu} cost_{tu}\right) \tag{5.1}$$

subject to

$$F_s = \sum_{tu} F_{s,tu}, \quad \forall s \in S \tag{5.2}$$

$$\sum_{s} F_{s,tu} + \sum_{tu'} F^{rec}_{tu',tu} = F^{in}_{tu}, \quad \forall tu \in TU \tag{5.3}$$

$$F^{in}_{tu} = F^{out}_{tu} + F^{loss}_{tu}, \quad \forall tu \in TU \tag{5.4}$$

$$F^{out}_{tu} = \sum_{tu'} F^{rec}_{tu,tu'} + \sum_{sgu} F^{exit}_{tu,sgu}, \quad \forall tu \in TU \tag{5.5}$$

$$F^{in}_{sgu} = \sum_{tu} F^{exit}_{tu,sgu}, \quad \forall sgu \in SGU \tag{5.6}$$

$$F^{in}_{sgu} = F^{out}_{sgu}, \quad \forall sgu \in SGU \tag{5.7}$$

$$\sum_{sgu} F^{out}_{sgu} = F^{in}_{WI} \tag{5.8}$$

$$F^{in}_{WI} = Demand^{steam} \tag{5.9}$$

$$F^{in}_{HRSG} = F^{out}_{HRSG} + F^{bbd,rec}_{HRSG} \tag{5.10a}$$

$$F^{in}_{DB} = F^{out}_{DB} + F^{bbd,rec}_{DB} \tag{5.10b}$$

$$\beta_{bbd} F^{in}_{OTSG} = F^{out}_{OTSG} \tag{5.10c}$$

$$(1 - \beta^{bbd}) F^{in}_{OTSG} = F^{bbd,rec}_{OTSG} \tag{5.10d}$$

$$F_{PW} = \beta^{emul} F^{in}_{WI} \tag{5.11a}$$

$$F_{MUW} = (1 - \beta^{emul}) F^{in}_{WI} + \sum_{tu} F^{loss}_{tu} \tag{5.11b}$$

$$F_{BBD} = \sum_{sgu} F^{bbd,rec}_{sgu} \tag{5.11c}$$

$$\sum_{s} B_{s,tu} + \sum_{tu'} B_{tu',tu} \leq NS^{max}, \quad \forall tu \in TU \tag{5.12}$$

$$B_{tu,tu'} + B_{tu',tu} \leq 1, \quad \forall tu, tu' \in TU \tag{5.13}$$

$$Bound^{up} = \sum_{s} F_s \tag{5.14}$$

$$B^{in}_{tu} = B^{out}_{tu}, \quad \forall tu \in TU \tag{5.15}$$

$$B^{in}_{sgu} = B^{out}_{sgu}, \quad \forall sgu \in SGU \tag{5.16}$$

$$B^{bbd,rec}_{OTSG} = B^{in}_{OTSG} \tag{5.17}$$

$$F_{s,tu} \leq B_{s,tu} Bound^{up}, \quad \forall s \in S, tu \in TU \tag{5.18a}$$

$$F_{s,tu} \geq B_{s,tu} Bound^{low}, \quad \forall s \in S, tu \in TU \tag{5.18b}$$

$$F^{rec}_{tu,tu'} \leq B_{tu,tu'} Bound^{up}, \quad \forall tu, tu' \in TU \tag{5.19a}$$

$$F^{rec}_{tu,tu'} \geq B_{tu,tu'} Bound^{low}, \quad \forall tu, tu' \in TU \tag{5.19b}$$

$$F^{in}_{tu} \leq B^{in}_{tu} Bound^{up}, \quad \forall tu \in TU \tag{5.20a}$$

$$F^{in}_{tu} \geq B^{in}_{tu} Bound^{low}, \quad \forall tu \in TU \tag{5.20b}$$

$$F^{out}_{tu} \leq B^{out}_{tu} Bound^{up}, \quad \forall tu \in TU \tag{5.21a}$$

$$F^{out}_{tu} \geq B^{out}_{tu} Bound^{low}, \quad \forall tu \in TU \tag{5.21b}$$

$$F^{exit}_{tu,sgu} \leq B^{exit}_{tu,sgu} Bound^{up}, \quad \forall tu \in TU, sgu \in SGU \tag{5.22a}$$

$$F^{exit}_{tu,sgu} \geq B^{exit}_{tu,sgu} Bound^{low}, \quad \forall tu \in TU, sgu \in SGU \tag{5.22b}$$

$$F^{in}_{sgu} \leq B^{in}_{sgu} Bound^{up}, \quad \forall sgu \in SGU \tag{5.23a}$$

$$F^{in}_{sgu} \geq B^{in}_{sgu} Bound^{low}, \quad \forall sgu \in SGU \tag{5.23b}$$

$$F^{out}_{sgu} \leq B^{out}_{sgu} Bound^{up}, \quad \forall sgu \in SGU \tag{5.24a}$$

$$F^{out}_{sgu} \geq B^{out}_{sgu} Bound^{low}, \quad \forall sgu \in SGU \tag{5.24b}$$

$$F^{bbd,rec}_{sgu} \leq B^{bbd,rec}_{sgu} Bound^{up}, \quad \forall sgu \in SGU \tag{5.25a}$$

$$F^{bbd,rec}_{sgu} \geq B^{bbd,rec}_{sgu} Bound^{low}, \quad \forall sgu \in SGU \tag{5.25b}$$

$$F_{WI}^{in} \leq B_{pro}^{in} Bound^{up} \tag{5.26a}$$

$$F_{WI}^{in} \geq B_{WI}^{in} Bound^{up} \tag{5.26b}$$

$$\sum_{s} F_{s,tu} C_{s,c} + \sum_{tu'} F_{tu',tu}^{rec} C_{tu',c}^{out} = F_{tu}^{in} C_{tu,c}^{in}, \quad \forall tu \in TU, c \in C \tag{5.27}$$

$$(1 - RR_{tu,c}) F_{tu}^{in} C_{tu,c}^{in} = F_{tu}^{out} C_{tu,c}^{out}, \quad \forall tu \in TU, c \in C \tag{5.28}$$

$$F_{tu}^{out} C_{tu,c}^{out} = \sum_{sgu} F_{tu,sgu}^{exit} C_{tu,c}^{out} + \sum_{tu'} F_{tu,tu'}^{rec} C_{tu,c}^{out}, \quad \forall tu \in TU, c \in C \tag{5.29}$$

$$\sum_{tu} F_{tu,sgu}^{exit} C_{tu,c}^{out} = F_{sgu}^{in} C_{sgu,c}^{in}, \quad \forall sgu \in SGU, c \in C \tag{5.30}$$

$$C_{tu,c}^{in} \leq C_{tu,c}^{max}, \quad \forall tu \in TU, c \in C \tag{5.31}$$

$$C_{sgu,c}^{in} \leq C_{sgu,c}^{target}, \quad \forall sgu \in SGU, c \in C \tag{5.32}$$

$$cost_s = cost_s^{fix} + HY(cost_s^{var}), \quad \forall s \in S \tag{5.33}$$

$$cost_{tu} = (a_{tu}^{fix} F_{tu}^{in} + b_{tu}^{fix}) + HY(a_{tu}^{var} F_{tu}^{in} + b_{tu}^{var}), \quad \forall tu \in TU \tag{5.34}$$

Table 5.1: Decision variables in the SAGD model

| Variable | Description | Associated design variable |
|---|---|---|
| | Flow variables (tonne/hr) | |
| $F_s$ | Source flow | |
| $F_{s,tu}$ | Exit flow from source splitter to treatment unit | $B_{s,tu}$ |
| $F_{tu}^{in}$ | Inflow to treatment unit | $B_{tu}^{in}$ |
| $F_{tu}^{out}$ | Outflow from treatment unit | $B_{tu}^{out}$ |
| $F_{tu,tu'}^{rec}$ | Recycle flow between treatment units | $B_{tu,tu'}^{rec}$ |
| $F_{tu,sgu}^{exit}$ | Exit flow from treatment unit to steam generation units | $B_{tu,sgu}^{exit}$ |
| $F_{sgu}^{in}$ | Inflow to steam generation unit | $B_{sgu}^{in}$ |
| $F_{sgu}^{out}$ | Outflow from steam generation unit | $B_{sgu}^{out}$ |
| $F_{sgu}^{bbd,rec}$ | Recycle flow from steam generation unit to source flow as boiler blowdown | $B_{sgu}^{bbd,rec}$ |
| $F_{WI}^{in}$ | Steam inflow for well injection | $B_{WI}^{in}$ |
| | Concentration variables (ppm) | |
| $C_{tu,c}^{in}$ | Concentration of contaminant in inflow to treatment unit | |
| $C_{tu,c}^{out}$ | Concentration of contaminant in outflow from treatment unit | |
| $C_{sgu,c}^{in}$ | Concentration of contaminant in inflow to steam generation unit | |

Table 5.2: Source water contaminant concentration ($C_{s,c}$ in ppm) in the SAGD model

| | $O$ | $Si$ | $TH$ | $TSS$ |
|---|---|---|---|---|
| $PW$ | 2000 | 350 | 20 | 50 |
| $MUW$ | 0 | 15 | 150 | 0 |
| $BBD$ | 10 | 150 | 1 | 1 |

Table 5.3: Treatment unit efficiency ($RR_{tu,c}$) in the SAGD model

| | $O$ | $Si$ | $TH$ | $TSS$ |
|---|---|---|---|---|
| $ST$ | 0.9 | 0 | 0 | 0.5 |
| $IGF$ | 0.9 | 0 | 0 | 0.7 |
| $ORF$ | 0.91 | 0 | 0 | 0.95 |
| $HCY$ | 0.93 | 0 | 0 | 0 |
| $LS$ | 0 | 0.9 | 0.5 | 0 |
| $EVAP$ | 0.99 | 0.99 | 0.99 | 0.99 |
| $WAC$ | 0 | 0 | 0.99 | 0 |

Table 5.4: Cost parameters for source water in the SAGD model

| | | $PW$ | $MUW$ | $BBD$ |
|---|---|---|---|---|
| $cost_s^{fix}$ | Fixed cost | 0 | 0 | 0 |
| $cost_s^{var}$ | Variable cost | 0 | $1.59 \times 10^{-6}$ | 0 |

Table 5.5: Cost parameters for treatment units in the SAGD model

| Parameters ($\times 10^{-6}$) | $ST$ | $IGF$ | $ORF$ | $HCY$ | $LS$ | $EVAP$ | $WAC$ |
|---|---|---|---|---|---|---|---|
| $a_{tu}^{fix}$ | 2989.5 | 1906.7 | 1248.9 | 3000 | 9705.5 | 28723 | 1550.9 |
| $b_{tu}^{fix}$ | 0 | 12292 | −401.99 | 50000 | −860733 | 12926 | −317.74 |
| $a_{tu}^{var}$ | 109.26 | 432.94 | 0 | 1 | 5388 | 15529 | 494.23 |
| $b_{tu}^{var}$ | 0 | 23585 | 0 | 1 | −479602 | 10626 | −31.142 |

Table 5.6: Auxiliary parameters in the SAGD model

| Parameters (units) | | | |
|---|---|---|---|
| $Bound^{low}$ | Lower bound on flow (tonne/hr) | | 10 |
| $NS^{max}$ | Maxiumum number of streams allowed into treatment units | | 9 |
| $\beta^{emul}$ | Bitumen emulsion separation ratio | | 0.95 |
| $\beta^{bbd}$ | Steam conversion efficiency of $OTSG$ | | 0.8 |
| $HY$ | Number of hours of operation of the plant (hr/yr) | | 8322 |
| $Demand^{steam}$ | Steam demand from the well injection site at nominal conditions (tonne/hr) | | 625 |
| $C^{max}_{tu,c}$ | Maximum allowable inlet concentration for all treatment units (ppm) | $O$ | 2500 |
| | | $Si$ | 400 |
| | | $TH$ | 400 |
| | | $TSS$ | 100 |
| $C^{target}_{sgu,c}$ | Target inlet concentration for all steam generation units (ppm) | $O$ | 10 |
| | | $Si$ | 150 |
| | | $TH$ | 1 |
| | | $TSS$ | 1 |

The deterministic model was solved on GAMS consecutively using the BARON MINLP solver [49], with the IPOPT NLP solver specification. The locally optimal objective magnitude at $\xi^* = 0.5$ was found to be 16110.5367, and the resulting optimal network is depicted in Figure 5.2. The solution selected only the $HRSG$ unit for steam generation, and therefore, the $BBD$ stream did not factor in this solution.

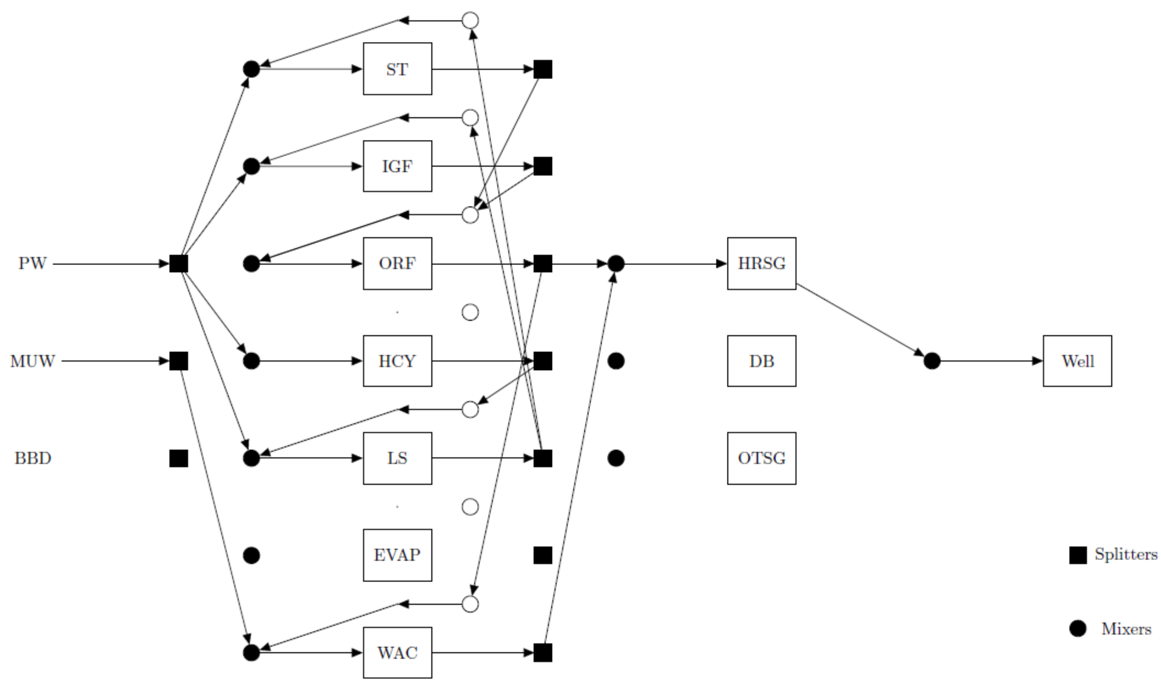


Figure 5.2: Optimal solution for the deterministic formulation of the SAGD model

## 5.3 Robust counterpart of nonlinear LDR-based formulation of SAGD model

The nonlinear robust optimization technique, discussed in Chapter 4 was applied to the SAGD model in Section 5.2 in a similar manner. In this model, the uncertainty was sourced from steam demand ($Demand^{steam}(\xi)$), and as a result, all the flow and concentration variables involved in the model were found to be dependent on uncertainty. In this problem, the uncertain steam demand ($Demand^{steam}(\xi)$) was modeled as follows,

$$Demand^{steam}(\xi) = \xi Demand^{low} + (1 - \xi)Demand^{high}$$

where $Demand^{low}$ and $Demand^{high}$ were taken to be the extreme points for the realizations of $Demand^{steam}$. The source flow was assumed to vary between 500 tonne/hr ($Demand^{low}$) and 750 tonne/hr ($Demand^{high}$).

Using the technique detailed in 4.1, the decision variables in the SAGD model were classified into decision, state and control variables, as shown in Table 5.7. The uncertain steam demand was modeled, as follows:

$$Demand^{steam}(\xi) = \xi Demand^{low} + (1 - \xi)Demand^{high} \tag{5.35}$$

The control variables in the model were reformulated using the affine decision rule, as follows:

$$F_{s,tu}(\xi) = F^0_{s,tu} + F^1_{s,tu}\xi, \quad \forall s \in S, tu \in TU, \xi \in \Xi \tag{5.36}$$

$$F^{rec}_{tu,tu'}(\xi) = F^{rec,0}_{tu,tu'} + F^{rec,1}_{tu,tu'}\xi, \quad \forall tu, tu' \in TU, \xi \in \Xi \tag{5.37}$$

$$F^{exit}_{tu,sgu}(\xi) = F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi, \quad \forall tu \in TU, \xi \in \Xi \tag{5.38}$$

The implicit derivatives of the state variables ($m(\xi)$) are denoted by $y_m$, while the first-order partial derivatives, with respect to uncertainty, of the inequality functions of flow limits are denoted by $\nabla_m$. The dual variables associated with the robust counterparts of the flow and concentration limits, and non-negativity constraints, are denoted by $\alpha_g$, where $g$ represents the inequality constraint that the dual is derived for. The decision rule parameters for the control variables that are optimized by this model are grouped into $F^0$ and $F^1$.

Table 5.7: Classification of variables in the nonlinear robust formulation of the SAGD model

| Design variables | State variables | Control variables |
|---|---|---|
| $B_{s,tu}$ | $F_s(\xi)$ | $F_{s,tu}(\xi)$ |
| $B^{in}_{tu}$ | $F^{in}_{tu}(\xi)$ | $F^{rec}_{tu,tu'}(\xi)$ |
| $B^{out}_{tu}$ | $F^{out}_{tu}(\xi)$ | $F^{exit}_{tu,sgu}(\xi)$ |
| $B^{rec}_{tu,tu'}$ | $F^{in}_{sgu}(\xi)$ | |
| $B^{exit}_{tu,sgu}$ | $F^{out}_{sgu}(\xi)$ | |
| $B^{in}_{sgu}$ | $F^{bbd,rec}_{sgu}(\xi)$ | |
| $B^{out}_{sgu}$ | $F^{in}_{WI}(\xi)$ | |
| $B^{bbd,rec}_{sgu}$ | $Bound^{up}(\xi)$ | |
| $B^{in}_{WI}$ | $C^{in}_{tu,c}(\xi)$ | |
| | $C^{out}_{tu,c}(\xi)$ | |
| | $C^{in}_{sgu,c}(\xi)$ | |

$$\min \quad \left(\sum_s cost_s\right) + \left(\sum_{tu} cost_{tu}\right) \tag{5.39}$$

subject to

$$F_s(\xi^*) - \left(\sum_{tu} F^0_{s,tu} + F^1_{s,tu}\xi^*\right) = 0, \quad \forall s \in S \qquad y_{F_s} - \sum_{tu} F^1_{s,tu} = 0, \quad \forall s \in S \tag{5.40a}$$

$$\left(\sum_{s} F^{0}_{s,tu} + F^{1}_{s,tu}\xi^*\right) + \left(\sum_{tu} F^{rec,0}_{tu',tu} + F^{rec,1}_{tu',tu}\xi^*\right) - F^{in}_{tu}(\xi^*) = 0, \quad \forall tu \in TU \tag{5.41a}$$

$$\left(\sum_{tu'} F^{rec,1}_{tu',tu}\right) + \left(\sum_{s} F^{1}_{s,tu}\right) - y_{F^{in}_{tu}} = 0, \quad \forall tu \in TU \tag{5.41b}$$

$$F^{in}_{tu}(\xi^*) - F^{out}_{tu}(\xi^*) - F^{loss}_{tu} = 0, \quad \forall tu \in TU \tag{5.42a}$$

$$y_{F^{in}_{tu}} - y_{F^{out}_{tu}} = 0, \quad \forall tu \in TU \tag{5.42b}$$

$$F^{out}_{tu}(\xi^*) - \left(\sum_{tu'} F^{rec,0}_{tu,tu'} + F^{rec,1}_{tu,tu'}\xi^*\right) - \left(\sum_{sgu} F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^*\right) = 0, \quad \forall tu \in TU \tag{5.43a}$$

$$y_{F^{out}_{tu}} - \sum_{tu'} F^{rec,1}_{tu,tu'} - \sum_{sgu} F^{exit,1}_{tu,sgu} = 0, \quad \forall tu \in TU \tag{5.43b}$$

$$F^{in}_{sgu}(\xi^*) - \left(\sum_{tu} F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^*\right) = 0, \quad \forall sgu \in SGU \tag{5.44a}$$

$$y_{F^{in}_{sgu}} - \sum_{tu} F^{exit,1}_{tu,sgu} = 0, \quad \forall sgu \in SGU \tag{5.44b}$$

$$F^{in}_{HRSG}(\xi^*) - F^{out}_{HRSG}(\xi^*) - F^{bbd,rec}_{HRSG}(\xi^*) = 0 \tag{5.45a}$$

$$y_{F^{in}_{HRSG}} - y_{F^{out}_{HRSG}} - y_{F^{bbd,rec}_{HRSG}} = 0 \tag{5.45b}$$

$$F^{in}_{DB}(\xi^*) - F^{out}_{DB}(\xi^*) - F^{bbd,rec}_{DB}(\xi^*) = 0 \tag{5.46a}$$

$$y_{F^{in}_{DB}} - y_{F^{out}_{DB}} - y_{F^{bbd,rec}_{DB}} = 0 \tag{5.46b}$$

$$\beta_{bbd} F^{in}_{OTSG}(\xi^*) - F^{out}_{OTSG}(\xi^*) = 0 \tag{5.47a}$$

$$\beta_{bbd} y_{F^{in}_{OTSG}} - y_{F^{out}_{OTSG}} = 0 \tag{5.47b}$$

$$(1 - \beta_{bbd}) F^{in}_{OTSG}(\xi^*) - F^{bbd,rec}_{OTSG}(\xi^*) = 0 \tag{5.48a}$$

$$\beta_{bbd} y_{F^{in}_{OTSG}} - y_{F^{bbd,rec}_{OTSG}} = 0 \tag{5.48b}$$

$$\left(\sum_{sgu} F^{out}_{sgu}(\xi^*)\right) - F^{in}_{WI}(\xi^*) = 0, \quad \forall sgu \in SGU \tag{5.49a}$$

$$y_{F^{out}_{sgu}} - y_{F^{in}_{WI}} = 0, \quad \forall sgu \in SGU \tag{5.49b}$$

$$\left(\sum_{sgu} F^{out}_{sgu}\right) - F^{in}_{WI}(\xi^*) = 0 \tag{5.50a}$$

$$\sum_{sgu} y_{F^{out}_{sgu}} - y_{F^{in}_{WI}} = 0 \tag{5.50b}$$

$$F_{PW}(\xi^*) - \beta_{emul} F_{WI}^{in}(\xi^*) = 0 \tag{5.51a}$$

$$y_{F_{PW}} - \beta_{emul} y_{F_{WI}^{in}} = 0 \tag{5.51b}$$

$$F_{MUW}(\xi^*) = (1 - \beta_{emul}) F_{WI}^{in}(\xi^*) + \sum_{tu} F_{tu}^{loss} = 0 \tag{5.52a}$$

$$y_{F_{MUW}} - (1 - \beta_{emul}) y_{F_{MUW}^{in}} = 0 \tag{5.52b}$$

$$F_{BBD}(\xi^*) - \sum_{sgu} F_{sgu}^{bbd,rec}(\xi^*) = 0 \tag{5.53a}$$

$$y_{F_{BBD}} - \sum_{sgu} y_{F_{sgu}^{bbd,rec}} = 0 \tag{5.53b}$$

$$\sum_{s} B_{s,tu} + \sum_{tu'} B_{tu',tu} \leq NS^{max}, \quad \forall tu \in TU \tag{5.54}$$

$$B_{tu,tu'} + B_{tu',tu} \leq 1, \quad \forall tu, tu' \in TU \tag{5.55}$$

$$B_{tu}^{in} = B_{tu}^{out}, \quad \forall tu \in TU \tag{5.56}$$

$$B_{sgu}^{in} = B_{sgu}^{out}, \quad \forall sgu \in SGU \tag{5.57}$$

$$B_{OTSG}^{bbd,rec} = B_{OTSG}^{in} \tag{5.58}$$

$$-\left(F_{s,tu}^{0} + F_{s,tu}^{1}\xi^* - B_{s,tu} Bound^{up}\right) + (\xi^* \nabla_{F_{s,tu}}) + b^\top \gamma_{F_{s,tu}} \geq 0, \quad \forall s \in S, tu \in TU \tag{5.59a}$$

$$A^\top \gamma_{F_{s,tu}} + \nabla_{F_{s,tu}} = 0, \quad \forall s \in S, tu \in TU \tag{5.59b}$$

$$\left(F_{s,tu}^{0} + F_{s,tu}^{1}\xi^* - B_{s,tu} Bound^{up}\right) + (\xi^* \nabla_{F_{s,tu}}) + b^\top \gamma_{F_{s,tu}} \geq 0, \quad \forall s \in S, tu \in TU \tag{5.59c}$$

$$A^\top \gamma_{F_{s,tu}} + \nabla_{F_{s,tu}} = 0, \quad \forall s \in S, tu \in TU \tag{5.59d}$$

$$-\left(F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1}\xi^* - B_{tu,tu'}^{rec} Bound^{up}\right) + (\xi^* \nabla_{F_{tu,tu'}^{rec}}) + b^\top \gamma_{F_{tu,tu'}^{rec}} \geq 0, \quad \forall tu, tu' \in TU \tag{5.60a}$$

$$A^\top \gamma_{F_{tu,tu'}^{rec}} + \nabla_{F_{tu,tu'}^{rec}} = 0, \quad \forall tu, tu' \in TU \tag{5.60b}$$

$$\left(F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1}\xi^* - B_{tu,tu'}^{rec} Bound^{up}\right) + (\xi^* \nabla_{F_{tu,tu'}^{rec}}) + b^\top \gamma_{F_{tu,tu'}^{rec}} \geq 0, \quad \forall tu, tu' \in TU \tag{5.60c}$$

$$A^\top \gamma_{F^{rec}_{tu,tu'}} + \nabla_{F^{rec}_{tu,tu'}} = 0, \quad \forall tu, tu' \in TU \tag{5.60d}$$

$$-\left(F^{in}_{tu}(\xi^*) - B^{in}_{tu} Bound^{up}\right) + (\xi^* \nabla_{F^{in}_{tu}}) + b^\top \gamma_{F^{in}_{tu}} \geq 0, \quad \forall tu \in TU \tag{5.61a}$$

$$A^\top \gamma_{F^{in}_{tu}} + \nabla_{F^{in}_{tu}} = 0, \quad \forall tu \in TU \tag{5.61b}$$

$$\left(F^{in}_{tu}(\xi^*) - B^{in}_{tu} Bound^{up}\right) + (\xi^* \nabla_{F^{in}_{tu}}) + b^\top \gamma_{F^{in}_{tu}} \geq 0, \quad \forall tu \in TU \tag{5.61c}$$

$$A^\top \gamma_{F^{in}_{tu}} + \nabla_{F^{in}_{tu}} = 0, \quad \forall tu \in TU \tag{5.61d}$$

$$-\left(F^{out}_{tu}(\xi^*) - B^{out}_{tu} Bound^{up}\right) + (\xi^* \nabla_{F^{out}_{tu}}) + b^\top \gamma_{F^{out}_{tu}} \geq 0, \quad \forall tu \in TU \tag{5.62a}$$

$$A^\top \gamma_{F^{out}_{tu}} + \nabla_{F^{out}_{tu}} = 0, \quad \forall tu \in TU \tag{5.62b}$$

$$\left(F^{out}_{tu}(\xi^*) - B^{out}_{tu} Bound^{up}\right) + (\xi^* \nabla_{F^{out}_{tu}}) + b^\top \gamma_{F^{out}_{tu}} \geq 0, \quad \forall tu \in TU \tag{5.62c}$$

$$A^\top \gamma_{F^{out}_{tu}} + \nabla_{F^{out}_{tu}} = 0, \quad \forall tu \in TU \tag{5.62d}$$

$$-\left(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^* - B^{exit}_{tu,sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{exit}_{tu,sgu}}) + b^\top \gamma_{F^{exit}_{tu,sgu}} \geq 0, \quad \forall tu \in TU, sgu \in SGU \tag{5.63a}$$

$$A^\top \gamma_{F^{exit}_{tu,sgu}} + \nabla_{F^{exit}_{tu,sgu}} = 0, \quad \forall tu \in TU, sgu \in SGU \tag{5.63b}$$

$$\left(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^* - B^{exit}_{tu,sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{exit}_{tu,sgu}}) + b^\top \gamma_{F^{exit}_{tu,sgu}} \geq 0, \quad \forall tu \in TU, sgu \in SGU \tag{5.63c}$$

$$A^\top \gamma_{F^{exit}_{tu,sgu}} + \nabla_{F^{exit}_{tu,sgu}} = 0, \quad \forall tu \in TU, sgu \in SGU \tag{5.63d}$$

$$-\left(F^{in}_{sgu}(\xi^*) - B^{in}_{sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{in}_{sgu}}) + b^\top \gamma_{F^{in}_{sgu}} \geq 0, \quad \forall sgu \in SGU \tag{5.64a}$$

$$A^\top \gamma_{F^{in}_{sgu}} + \nabla_{F^{in}_{sgu}} = 0, \quad \forall sgu \in SGU \tag{5.64b}$$

$$\left(F^{in}_{sgu}(\xi^*) - B^{in}_{sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{in}_{sgu}}) + b^\top \gamma_{F^{in}_{sgu}} \geq 0, \quad \forall sgu \in SGU \tag{5.64c}$$

$$A^\top \gamma_{F^{in}_{sgu}} + \nabla_{F^{in}_{sgu}} = 0, \quad \forall sgu \in SGU \tag{5.64d}$$

$$-\left(F^{out}_{sgu}(\xi^*) - B^{out}_{sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{out}_{sgu}}) + b^\top \gamma_{F^{out}_{sgu}} \geq 0, \quad \forall sgu \in SGU \tag{5.65a}$$

$$A^\top \gamma_{F^{out}_{sgu}} + \nabla_{F^{out}_{sgu}} = 0, \quad \forall sgu \in SGU \tag{5.65b}$$

$$\left(F^{out}_{sgu}(\xi^*) - B^{out}_{sgu} Bound^{up}\right) + (\xi^* \nabla_{F^{out}_{sgu}}) + b^\top \gamma_{F^{out}_{sgu}} \geq 0, \quad \forall sgu \in SGU \tag{5.65c}$$

$$A^\top \gamma_{F^{out}_{sgu}} + \nabla_{F^{out}_{sgu}} = 0, \quad \forall sgu \in SGU \tag{5.65d}$$

$$-\left(F_{sgu}^{bbd,rec}(\xi^*) - B_{sgu}^{bbd,rec}Bound^{up}\right) + (\xi^*\nabla_{F_{sgu}^{bbd,rec}}) + b^\top\gamma_{F_{sgu}^{bbd,rec}} \geq 0, \quad \forall sgu \in SGU \tag{5.66a}$$

$$A^\top\gamma_{F_{sgu}^{bbd,rec}} + \nabla_{F_{sgu}^{bbd,rec}} = 0, \quad \forall sgu \in SGU \tag{5.66b}$$

$$\left(F_{sgu}^{bbd,rec}(\xi^*) - B_{sgu}^{bbd,rec}Bound^{up}\right) + (\xi^*\nabla_{F_{sgu}^{bbd,rec}}) + b^\top\gamma_{F_{sgu}^{bbd,rec}} \geq 0, \quad \forall sgu \in SGU \tag{5.66c}$$

$$A^\top\gamma_{F_{sgu}^{bbd,rec}} + \nabla_{F_{sgu}^{bbd,rec}} = 0, \quad \forall sgu \in SGU \tag{5.66d}$$

$$-\left(F_{WI}^{in}(\xi^*) - B_{WI}^{in}Bound^{up}\right) + (\xi^*\nabla_{F_{WI}^{in}}) + b^\top\gamma_{F_{WI}^{in}} \geq 0 \tag{5.67a}$$

$$A^\top\gamma_{F_{WI}^{in}} + \nabla_{F_{WI}^{in}} = 0 \tag{5.67b}$$

$$-\left(F_{WI}^{in}(\xi^*) - B_{WI}^{in}Bound^{up}\right) + (\xi^*\nabla_{F_{WI}^{in}}) + b^\top\gamma_{F_{WI}^{in}} \geq 0 \tag{5.67c}$$

$$A^\top\gamma_{F_{WI}^{in}} + \nabla_{F_{WI}^{in}} = 0 \tag{5.67d}$$

$$\left(\sum_s (F_{s,tu}^0 + F_{s,tu}^1\xi^*)C_{s,c}\right) + \left(\sum_{tu'} (F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1}\xi^*)C_{tu,c}^{out}(\xi^*)\right) - F_{tu}^{in}(\xi^*)C_{tu,c}^{in}(\xi^*) = 0, \quad \forall tu \in TU, c \in C \tag{5.68a}$$

$$\sum_s F_{s,tu}^1 C_{s,c} + \sum_{tu'} F_{tu',tu}^{rec,1} C_{tu,c}^{out}(\xi^*) - (F_{tu}^{in}(\xi^*)y_{C_{tu,c}^{in}} + C_{tu,c}^{in}(\xi^*)y_{F_{tu}^{in}}) + \sum_{tu'} (F_{tu',tu}^{rec,0} + F_{tu',tu}^{rec,1}\xi^*)y_{C_{tu,c}^{out}} = 0, \quad \forall tu \in TU, c \in C \tag{5.68b}$$

$$(1 - RR_{tu,c})F_{tu}^{in}(\xi^*)C_{tu,c}^{in}(\xi^*) - F_{tu}^{out}(\xi^*)C_{tu,c}^{out}(\xi^*) = 0, \quad \forall tu \in TU, c \in C \tag{5.69a}$$

$$(1 - RR_{tu,c})(F_{tu}^{in}(\xi^*)y_{C_{tu,c}^{in}} + C_{tu,c}^{in}(\xi^*)y_{F_{tu}^{in}}) - (F_{tu}^{out}(\xi^*)y_{C_{tu,c}^{out}} + C_{tu,c}^{out}(\xi^*)y_{F_{tu}^{out}}) = 0, \quad \forall tu \in TU, c \in C \tag{5.69b}$$

$$F_{tu}^{out}(\xi^*)C_{tu,c}^{out}(\xi^*) - \left(\sum_{sgu} C_{tu,c}^{out}(\xi^*)(F_{tu,sgu}^{exit,0} + F_{tu,sgu}^{exit,1}\xi^*)\right) - \left(\sum_{tu'} C_{tu,c}^{out}(\xi^*)(F_{tu,tu'}^{rec,0} + F_{tu,tu'}^{rec,1}\xi^*)\right), \quad \forall tu \in TU, c \in C \tag{5.70a}$$

$$F^{out}_{tu}(\xi^*)y_{C^{out}_{tu,c}} + C^{out}_{tu,c}(\xi^*)y_{F^{out}_{tu}} - \left(\sum_{sgu} y_{C^{out}_{tu,c}}(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^*)\right)$$
$$- \left(\sum_{tu'} y_{C^{out}_{tu,c}}(F^{rec,0}_{tu,tu'} + F^{rec,1}_{tu,tu'}\xi^*)\right) - \sum_{sgu} F^{exit,1}_{tu,sgu}C^{out}_{tu,c}(\xi^*)$$
$$- \sum_{tu'} F^{rec,1}_{tu,tu'}C^{out}_{tu,c}(\xi^*) = 0, \quad \forall tu \in TU, c \in C \quad (5.70b)$$

$$\left(\sum_{tu} C^{out}_{tu,c}(\xi^*)(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^*)\right) - F^{in}_{sgu}(\xi^*)C^{in}_{sgu,c}(\xi^*) = 0,$$
$$\forall sgu \in SGU, c \in C \quad (5.71a)$$

$$\left(\sum_{tu} y_{C^{out}_{tu,c}}(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}\xi^*) + F^{exit,1}_{tu,sgu}C^{out}_{tu,c}(\xi^*)\right) -$$
$$(y_{C^{in}_{sgu,c}}F^{in}_{sgu}(\xi^*) + y_{F^{in}_{sgu}}C^{in}_{sgu,c}(\xi^*)) = 0, \quad \forall sgu \in SGU, c \in C \quad (5.71b)$$

$$\xi^*\nabla_{C^{in}_{tu,c}} - (C^{in}_{tu,c}(\xi^*) - C^{max}_{tu,c}) + b^\top\lambda_{C^{in}_{tu,c}} \geq 0, \quad \forall tu \in TU, c \in C \quad (5.72a)$$

$$A^\top\lambda_{C^{in}_{tu,c}} + \nabla_{C^{in}_{tu,c}} = 0, \quad \forall tu \in TU, c \in C \quad (5.72b)$$

$$\xi^*\nabla_{C^{in}_{sgu,c}} - (C^{in}_{sgu,c}(\xi^*) - C^{target}_{sgu,c}) + b^\top\lambda_{C^{in}_{sgu,c}} \geq 0, \quad \forall sgu \in SGU, c \in C \quad (5.73a)$$

$$A^\top\lambda_{C^{in}_{sgu,c}} + \nabla_{C^{in}_{sgu,c}} = 0, \quad \forall sgu \in SGU, c \in C \quad (5.73b)$$

$$F^{in}_{WI}(\xi^*) - \xi^* Demand^{low} - (1-\xi^*)Demand^{high} = 0 \quad (5.74a)$$

$$y_{F^{in}_{WI}} - (Demand^{low} - Demand^{high}) = 0 \quad (5.74b)$$

$$F^0_{s,tu} + b^\top\alpha_{F_{s,tu}} \geq 0, \quad s \in S, tu \in TU \quad (5.75a)$$
$$A^\top\alpha_{F_{s,tu}} = F^1_{s,tu}, \quad s \in S, tu \in TU \quad (5.75b)$$

$$F^{rec,0}_{tu,tu'} + b^\top\alpha_{F^{rec}_{tu,tu'}} \geq 0, \quad tu, tu' \in TU \quad (5.76a)$$
$$A^\top\alpha_{F^{rec}_{tu,tu'}} = F^{rec,1}_{tu,tu'}, \quad tu, tu' \in TU \quad (5.76b)$$

$$F^{exit,0}_{tu,sgu} + b^\top\alpha_{F^{exit}_{tu,sgu}} \geq 0, \quad tu \in TU, sgu \in SGU \quad (5.77a)$$
$$A^\top\alpha_{F^{exit}_{tu}} = F^{exit,1}_{tu}, \quad tu \in TU, sgu \in SGU \quad (5.77b)$$

$$cost_s = cost^{fix}_s + HY(cost^{var}_s F_s(\xi^*)), \quad \forall s \in S \quad (5.78)$$
$$cost_{tu} = (a^{fix}_{tu}F^{in}_{tu}(\xi^*) + b^{fix}_{tu}) + HY(a^{var}_{tu}F^{in}_{tu}(\xi^*) + b^{var}_{tu}), \quad \forall tu \in TU \quad (5.79)$$

The nonlinear robust LDR model was derived around the nominal condition, i.e., $\xi^* = 0.5$, where the objective function was minimized for $\xi^*$. The model was derived for different ranges of uncertainty, $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$, and was solved in two stages. In the first stage, the decision and state variables were fixed using the locally optimal deterministic solution obtained in Section 5.2, using the BARON MINLP solver [49], with the IPOPT NLP solver specification. In the second stage, the model was re-solved after relaxing the bounds on the decision and state variables, using the ANTIGONE MINLP solver. The model was found to retain the deterministic decision and state variable solution for the nominal condition, and the locally optimal objective at $\xi^* = 0.5$ was found to be 16110.5367 for both ranges. An example of the resulting network is depicted for $\xi = 0.53$, using the LDR solution for $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$, in Figures 5.3 and 5.4, and the computed concentration profiles for $C^{in}_{sgu,c}$ for both ranges of uncertainty are shown in Figure 5.5. The optimal decision rule parameter for the control variables in the model are given in Table 5.8.

It was observed that when the nonlinear robust LDR model was solved for either range of uncertainty, the computed concentration profiles for $C^{in}_{HRSG,c}$ violated the targets (Table 5.6). The profiles were observed to be monotonically decreasing in nature. It was inferred that the violation of the target occurs as a result of using an approximate linearized model, and therefore, the decision rules obtained were deemed unsuitable for the operation of the system.

Table 5.8: Decision rule parameters for the control variables in the nonlinear robust LDR formulation of the SAGD model

| | $\xi \in [0.4, 0.6]$ | $\xi \in [0, 1]$ |
|---|---|---|
| $F_{PW,ST}$ | 233.8294 - 237.5$\xi$ | 230.1587 - 230.1587$\xi$ |
| $F_{PW,IGF}$ | 115.0794 | 116.9147 - 3.6706$\xi$ |
| $F_{PW,HCY}$ | 265.0836 | 265.0836 - 2.2737$\xi$ |
| $F_{PW,LS}$ | 98.5076 | 100.343 - 3.6706$\xi$ |
| $F_{MUW,WAC}$ | 37.5 - 12.5$\xi$ | 37.5 - 12.5$\xi$ |
| $F^{rec}_{ST,ORF}$ | 478.125 - 237.5$\xi$ | 474.4544 - 230.1587$\xi$ |
| $F^{rec}_{IGF,ORF}$ | 234.375 | 238.0456 - 7.3413$\xi$ |
| $F^{rec}_{ORF,WAC}$ | 554.5391 + 6.25$\xi$ | 666.5197 - 217.7113$\xi$ |
| $F^{rec}_{HCY,LS}$ | 265.0836 | 265.0836 |
| $F^{rec}_{LS,ST}$ | 244.2956 | 244.296 |
| $F^{rec}_{LS,IGF}$ | 119.2956 | 121.131 - 3.6706$\xi$ |
| $F^{exit}_{ORF,HRSG}$ | 157.9609 | 45.9803 - 19.7887$\xi$ |
| $F^{exit}_{WAC,HRSG}$ | 592.0391 | 704.0197 - 230.2113$\xi$ |

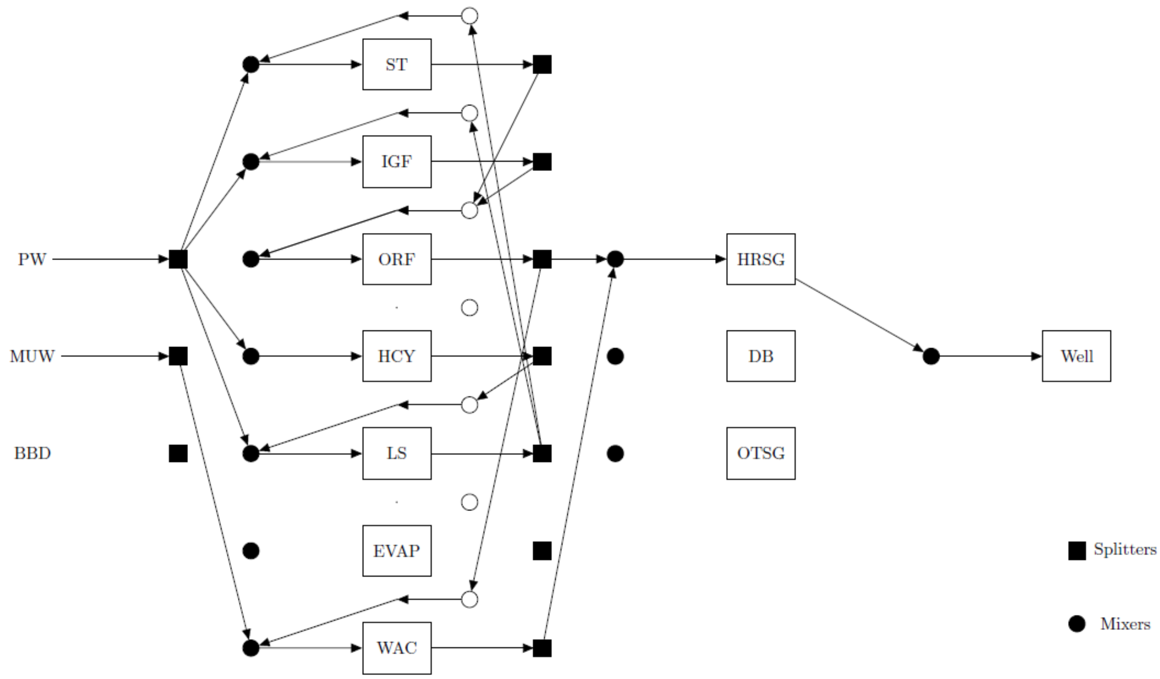


Figure 5.3: Optimal solution for the nonlinear robust LDR formulation of the SAGD model for $\xi \in [0.4, 0.6]$ at $\xi^* = 0.53$

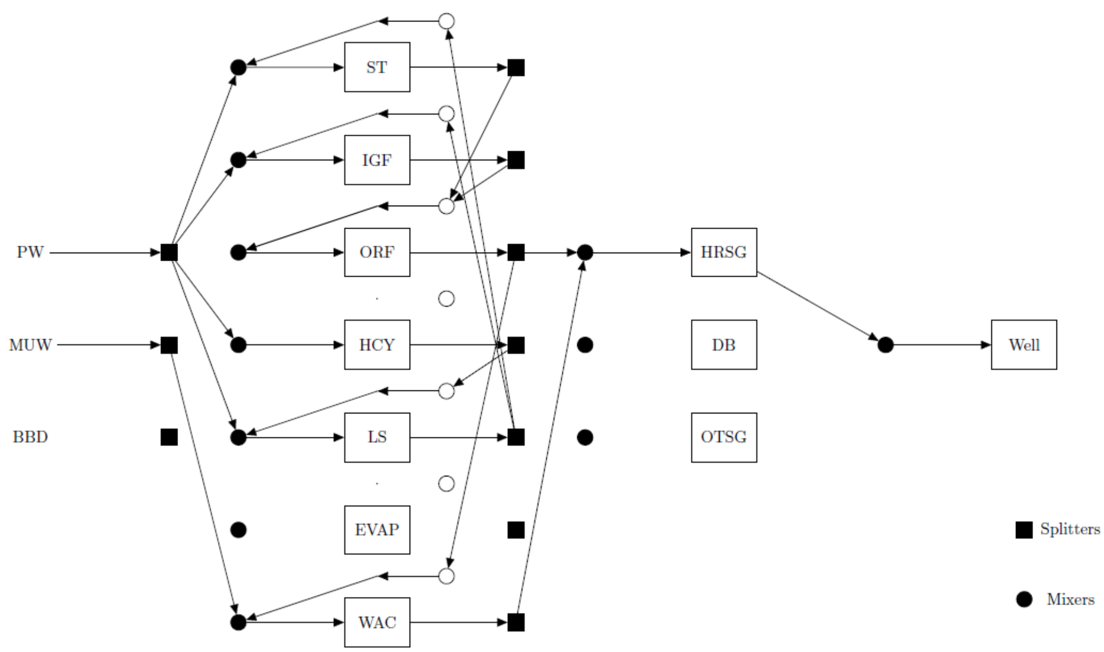


Figure 5.4: Optimal solution for the nonlinear robust LDR formulation of the SAGD model for $\xi \in [0, 1]$ at $\xi^* = 0.53$

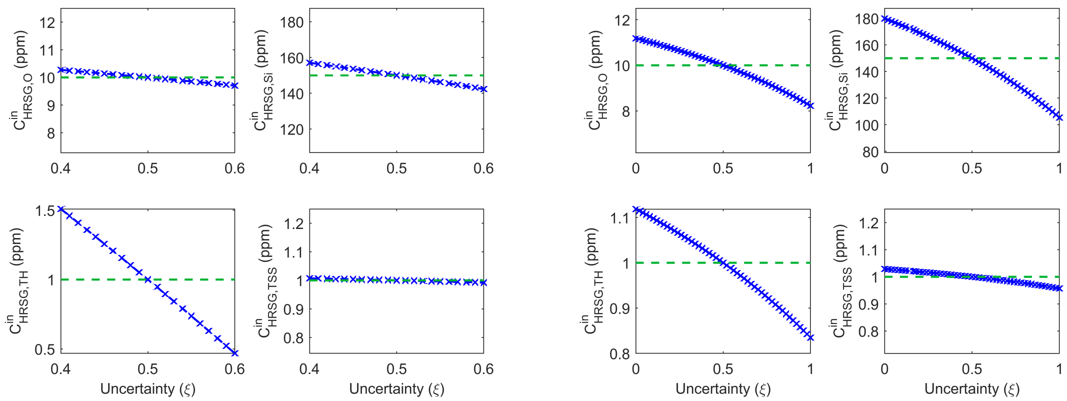

Figure 5.5: Computed concentration profiles of contaminants in inflow to the $HRSG$ using the decision rules from nonlinear robust LDR models for $\xi \in [0.4, 0.6]$ (left), and $\xi \in [0, 1]$ (right)

## 5.4 Proposed algorithm for improved solution to LDR model

In order to address the violation in target resulting from the linearization of the model around uncertainty, the following two-step approach was adopted.

*Step 1*: Obtaining a feasible solution to the model
(i) Beginning with the original targets $C_{sgu,c}^{target}$, pre-solve the deterministic model, followed by the robust LDR model.
(ii) Iteratively solve step 1(i) for increasingly stricter targets until a set of feasible decision rules is obtained.

*Step 2*: Improving the nonlinear robust LDR model
(i) Use the set of feasible decision rules from step 1(ii) as a starting solution for the improved LDR model (enforcing additional constraints at terminal points of uncertainty) to obtain improved decision rules.

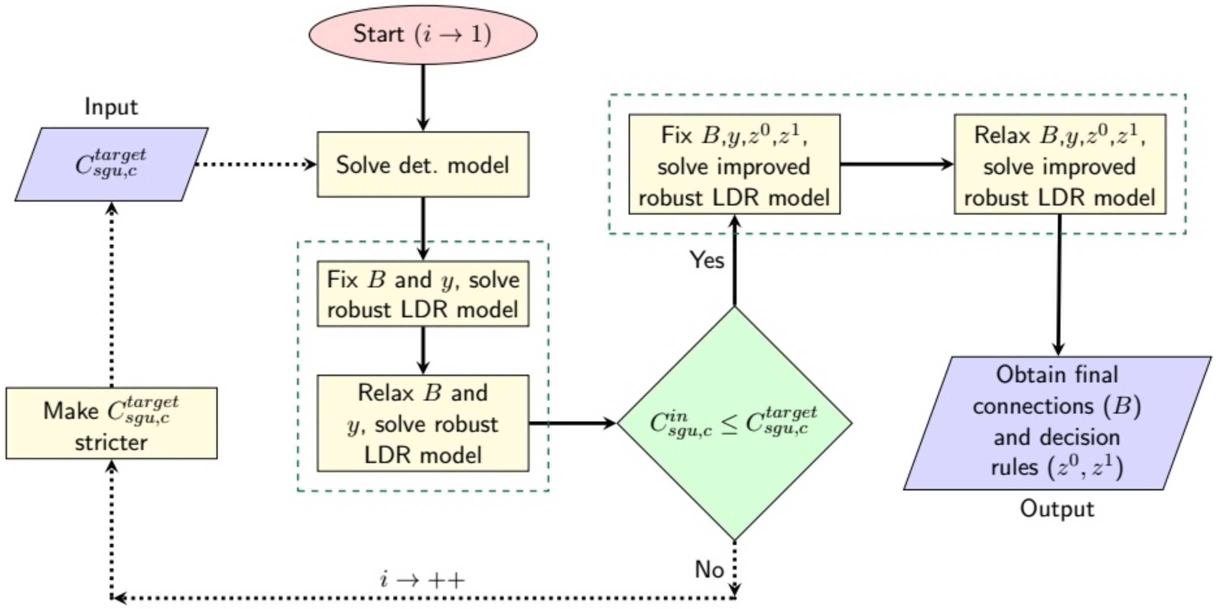


Figure 5.6: Flow representation of the improved nonlinear robust LDR model solution procedure

## 5.5 Robust counterpart of improved nonlinear LDR-based formulation of SAGD model

The solution procedure illustrated in Figure 5.6 was applied on the SAGD model. The deterministic model was solved for stricter targets - 8, 142, 0.6 and 0.85 ppm for $\xi \in [0.4, 0.6]$, and 8.8, 117, 0.72, 0.72 pm for $\xi \in [0, 1]$ for $O$, $Si$, $TH$ and $TSS$ respectively - using fixed steam generation unit connections from the deterministic solution in Section 5.2. The model was solved on GAMS consecutively using the BARON MINLP solver [49], with the IPOPT NLP solver specification. The locally optimal objective magnitude at $\xi^* = 0.5$ was found to be 17183.1551 for $\xi \in [0.4, 0.6]$ and 19707.43 for $\xi \in [0, 1]$.

The nonlinear robust LDR model in Section 5.3 was re-solved for the same stricter targets for both ranges of uncertainty, $\xi \in [0.4, 0.6]$ and $\xi \in [0, 1]$, using the same solver configuration, and the new deterministic solution. The resulting optimal solution was found to be feasible, with no violation of $C_{sgu,c}^{in}$. This solution was used to solve the modified nonlinear robust LDR model. The model in Section 5.3 was improved by adding terminal enforcement constraints, i.e., by enforcing the target concentration limits at the terminal realizations of uncertainty considered in the model. To formulate this improved model, the constraints given by Equations 5.2 - 5.2, 5.2, 5.2 - 5.11, 5.2 - 5.2, 5.2 and 5.2 were added to the model structure in Section 5.3, specific to each terminal realization of uncertainty. The modified LDR model is given as follows.

min [Equation 5.39]

subject to

[Equations 5.40a - 5.79]

$$F_{s,X} = \left( \sum_{tu} F^0_{s,tu} + F^1_{s,tu} X \right), \quad \forall s \in S, X \in \{\xi^{low}, \xi^{high}\} \tag{5.80}$$

$$\left( \sum_{tu} F^0_{s,tu} + F^1_{s,tu} X \right) + \left( \sum_{tu'} F^{rec,0}_{tu',tu} + F^{rec,1}_{tu',tu} X \right) = F^{in}_{tu,X}, \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \tag{5.81}$$

$$F^{in}_{tu,X} = F^{out}_{tu,X} + F^{loss}_{tu}, \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \tag{5.82}$$

$$F^{out}_{tu,X} = \left( \sum_{tu'} F^{rec,0}_{tu',tu} + F^{rec,1}_{tu',tu} X \right) + \left( \sum_{sgu} F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu} X \right), \quad \forall tu \in TU, X \in \{\xi^{low}, \xi^{high}\} \tag{5.83}$$

$$F^{in}_{sgu,X} = \left( \sum_{sgu} F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu} X \right), \quad \forall sgu \in SGU, X \in \{\xi^{low}, \xi^{high}\} \tag{5.84}$$

$$F^{in}_{sgu,X} = F^{out}_{sgu,X}, \quad \forall sgu \in SGU, X \in \{\xi^{low}, \xi^{high}\} \tag{5.85}$$

$$\sum_{sgu} F^{out}_{sgu,X} = F^{in}_{WI,X}, X \in \{\xi^{low}, \xi^{high}\} \tag{5.86}$$

$$F^{in}_{WI,X} = X Demand^{low} + (1 - X) Demand^{high}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.87}$$

$$F^{in}_{HRSG,X} = F^{out}_{HRSG,X} + F^{bbd,rec}_{HRSG}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.88a}$$

$$F^{in}_{DB,X} = F^{out}_{DB,X} + F^{bbd,rec}_{DB,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.88b}$$

$$\beta_{bbd} F^{in}_{OTSG,X} = F^{out}_{OTSG,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.88c}$$

$$(1 - \beta^{bbd}) F^{in}_{OTSG,X} = F^{bbd,rec}_{OTSG,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.88d}$$

$$F_{PW,X} = \beta^{emul} F^{in}_{WI,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.89a}$$

$$F_{MUW,X} = (1-\beta^{emul})F^{in}_{WI,X} + \sum_{tu} F^{loss}_{tu}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.89b}$$

$$F_{BBD,X} = \sum_{sgu} F^{bbd,rec}_{sgu,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.89c}$$

$$Bound^{up}_{X} = \sum_{s} F_{s,X}, \quad \forall X \in \{\xi^{low}, \xi^{high}\} \tag{5.90}$$

$$\sum_{s}(F^{0}_{s,tu} + F^{1}_{s,tu}X)C_{s,c} + \sum_{tu'}(F^{rec,0}_{tu',tu} + F^{rec,1}_{tu',tu}X)C^{out}_{tu',c,X} = F^{in}_{tu,X}C^{in}_{tu,c,X}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.91}$$

$$(1-RR_{tu,c})F^{in}_{tu,X}C^{in}_{tu,c,X} = F^{out}_{tu,X}C^{out}_{tu,c,X}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.92}$$

$$F^{out}_{tu,X}C^{out}_{tu,c,X} = \sum_{sgu}(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}X)C^{out}_{tu,c,X} + \sum_{tu'}(F^{rec,0}_{tu',tu} + F^{rec,1}_{tu',tu}X)C^{out}_{tu,c,X}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.93}$$

$$\sum_{tu}(F^{exit,0}_{tu,sgu} + F^{exit,1}_{tu,sgu}X)C^{out}_{tu,c,X} = F^{in}_{sgu,X}C^{in}_{sgu,c,X}, \quad \forall sgu \in SGU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.94}$$

$$C^{in}_{tu,c,X} \leq C^{max}_{tu,c}, \quad \forall tu \in TU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.95}$$

$$C^{in}_{sgu,c,X} \leq C^{target}_{sgu,c}, \quad \forall sgu \in SGU, c \in C, X \in \{\xi^{low}, \xi^{high}\} \tag{5.96}$$

This model was solved for the original targets, in two stages using the same solver configuration as Section 5.3. The locally optimal objective magnitude at $\xi^* = 0.5$ was found to be 16011.7631 for $\xi \in [0.4, 0.6]$ and 16589.5105 for $\xi \in [0, 1]$. An example of the resulting network is depicted for $\xi = 0.53$, using the LDR solution for $\xi \in [0.4, 0.6]$ in Figures 5.7 and 5.8, and the computed concentration profiles for $C^{in}_{sgu,c}$ for both ranges of uncertainty are shown in Figure 5.9. The optimal decision rule parameters for the control variables in the modified LDR model are given in Table 5.9.

Comparative plots of the evolution of the optimal objective magnitude profile, over the different ranges of uncertainty using the nonlinear robust LDR for original constraints, contrasted with the profiles obtained using the modified robust LDR model, using the approach detailed in Section 4.2, are illustrated in Figure 5.10. From the plots, it is evident that the solution of the modified nonlinear robust LDR-based model provided a feasible solution over the entire range of uncertainty considered in the model. The proposed algorithm, using the nonlinear robust optimization scheme with the affine decision rule, proved to give a feasible solution over the entire range of uncertainty, adjustable to its realization.

Table 5.9: Decision rule parameters for the control variables in the modified nonlinear robust LDR formulation of the SAGD model

| | $\xi \in [0.4, 0.6]$ | | $\xi \in [0, 1]$ |
|---|---|---|---|
| $F_{PW,ORF}$ | 712.5 - 237.5$\xi$ | $F_{PW,ORF}$ | 276.1905 - 92.0635$\xi$ |
| $F_{MUW,WAC}$ | 37.5 - 12.5$\xi$ | $F_{PW,LS}$ | 436.3095 - 145.4365$\xi$ |
| $F^{rec}_{ST,IGF}$ | 183.9488 - 82.8976$\xi$ | $F_{MUW,WAC}$ | 37.5 - 12.5$\xi$ |
| $F^{rec}_{ST,WAC}$ | 395.0619 | $F^{rec}_{IGF,WAC}$ | 328.7037 - 109.5679$\xi$ |
| $F^{rec}_{IGF,WAC}$ | 236.6627 - 168.3254$\xi$ | $F^{rec}_{ORF,IGF}$ | 372.0068 - 124.0023$\xi$ |
| $F^{rec}_{ORF,ST}$ | 228.8408 - 37.3641$\xi$ | $F^{rec}_{ORF,WAC}$ | 340.4932 - 113.4977$\xi$ |
| $F^{rec}_{ORF,HCY}$ | 446.3095 - 145.4365$\xi$ | $F^{rec}_{LS,ORF}$ | 436.3095 - 145.4365$\xi$ |
| $F^{rec}_{ORF,WAC}$ | 37.3497 - 54.6994$\xi$ | $F^{rec}_{WAC,ST}$ | 706.6969 - 235.5656$\xi$ |
| $F^{rec}_{HCY,ST}$ | 10 | $F^{exit}_{ST,HRSG}$ | 706.6969 - 235.5656$\xi$ |
| $F^{rec}_{HCY,LS}$ | 436.3095 - 145.4365$\xi$ | $F^{exit}_{IGF,HRSG}$ | 43.3031 - 14.4344$\xi$ |
| $F^{rec}_{LS,ST}$ | 383.5956 - 60.0087$\xi$ | | |
| $F^{rec}_{LS,IGF}$ | 52.7139 - 85.4278$\xi$ | | |
| $F^{exit}_{ST,HRSG}$ | 43.4257 - 14.4752$\xi$ | | |
| $F^{exit}_{WAC,HRSG}$ | 706.5743 - 235.5248$\xi$ | | |

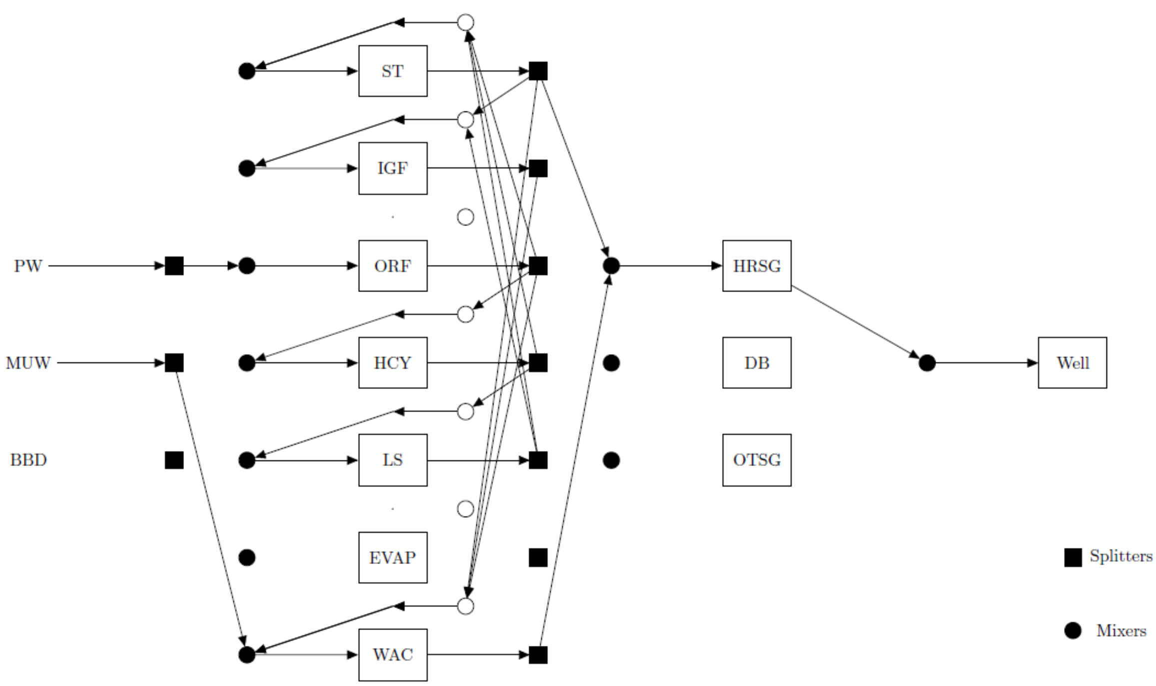


Figure 5.7: Optimal solution for the modified nonlinear robust LDR formulation of the SAGD model for $\xi \in [0.4, 0.6]$ at $\xi^* = 0.53$

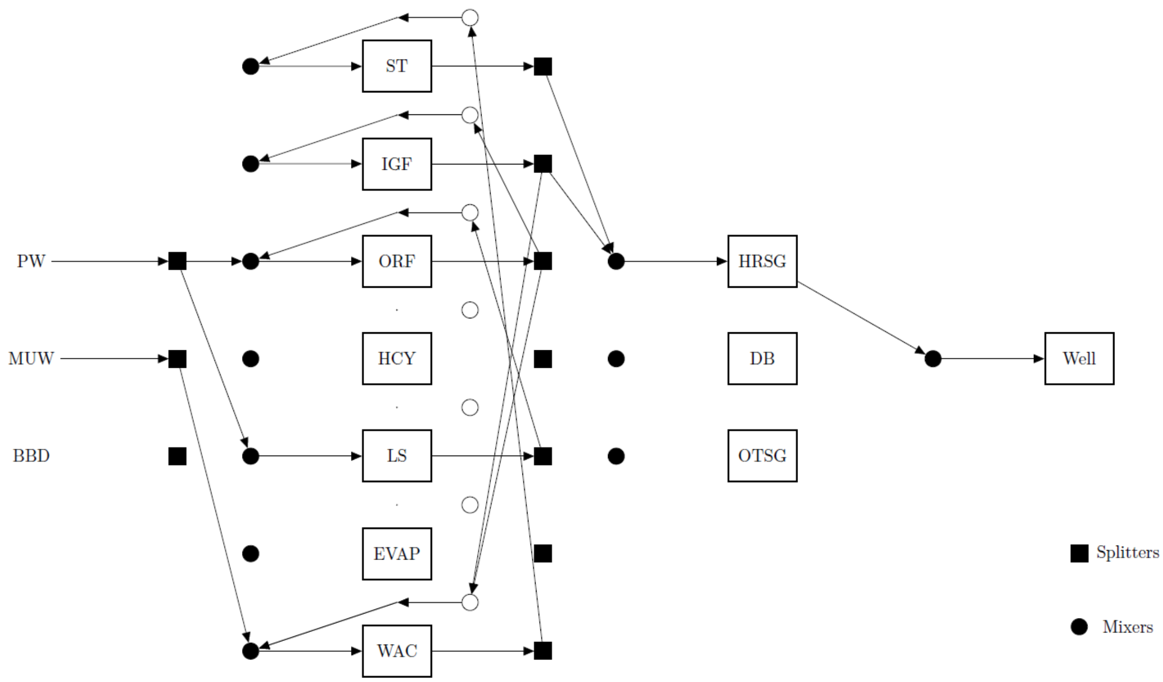


Figure 5.8: Optimal solution for the modified nonlinear robust LDR formulation of the SAGD model for $\xi \in [0, 1]$ at $\xi^* = 0.53$

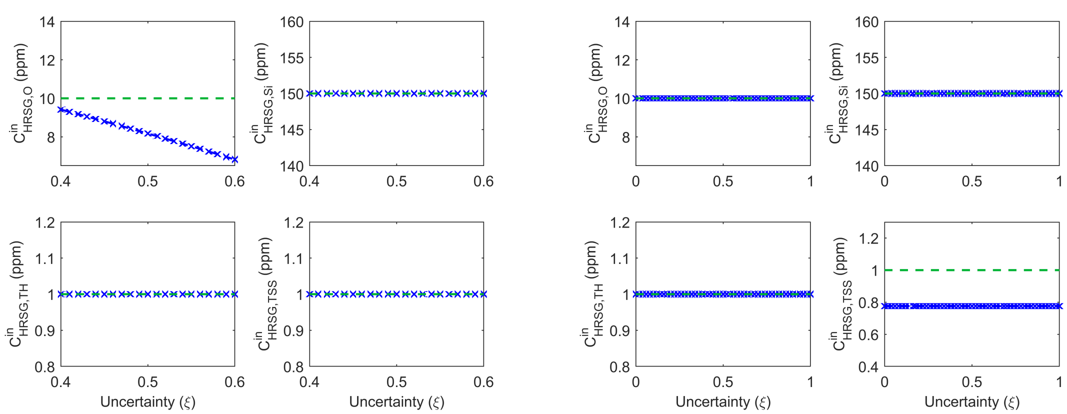


Figure 5.9: Computed concentration profiles of contaminants in inflow to the $HRSG$ using the decision rules from modified nonlinear robust LDR models for $\xi \in [0.4, 0.6]$ (left), and $\xi \in [0, 1]$ (right)

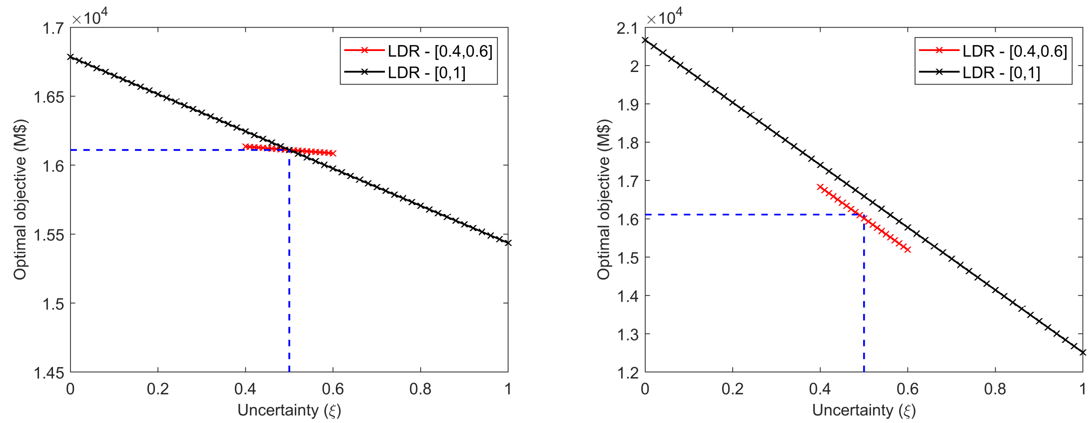


Figure 5.10: A comparative evolution of the optimal objective magnitude profile using the nonlinear robust model for original targets (left) and the modified robust model (right)

## 5.6 Concluding remarks

This chapter presented the application of the two-stage nonlinear robust optimization technique developed by Yuan, et al. [46] on the SAGD effluent treatment and steam generation network. Since the SAGD model was formulated as a large-scale MINLP problem, the model needed to be initialized with a feasible solution at each stage. As in the case of the small water treatment model, when the robust LDR model was solved, violations in the target concentration for the steam generation units were observed. Therefore, an alternative algorithm, similar to the scheme proposed for the small water treatment model, was developed for the SAGD MINLP model. Using the solution from the modified LDR model, it was observed that the decision rules successfully provided feasible solutions with respect to target concentrations, as well as flow and component balances, for the entire range of uncertainty.

# Chapter 6

# Summary and Future Work

## 6.1 Summary

In this thesis, the application of different variants of decision-rule based optimization for the optimal design and operation of effluent treatment systems was evaluated. Two case studies were chosen for analysis - a small water treatment model, and the effluent treatment-cum-steam generation model for a SAGD reservoir. All preliminary evaluations were conducted for the simple water treatment model. Initially, due to the bilinear nature of certain constraints in the models, the need to obtain linear models for the purpose of obtaining a robust counterpart was recognized. The first method of linearization utilized McCormick bounding envelopes to obtain the relaxed formulation of the original nonlinear model. The solution obtained through solving the relaxed LP model under uncertainty, using the affine decision rule formulation, proved to be infeasible due to violation of component balance constraints throughout the network. The second method of linearization used the optimal solution obtained at the nominal conditions to linearize the bilinear terms in the NLP model, using first order Taylor series approximation. The solution obtained through solving the linearized model under uncertainty, too, proved to be infeasible due to similar component balance violations, due to inadequate linearization.

In order to address the issues of infeasibility due to improper linearization, the nonlinear robust optimal design procedure, developed by Yuan, et al. (2018) [46] was applied on the model. The solution obtained through this technique provided a feasible solution for all ranges of uncertainty considered in the model, through a set of decision rules for all control variables. This technique was further applied to a larger case study - the effluent treatment system for the SAGD model. An algorithm to improve the performance of the nonlinear robust optimization technqiue, was proposed to obtain a better feasible solution. The final set of decision rules obtained for the control variables offered a feasible solution for all realizations of uncertainty considered in the model. Thus, the application of two-stage nonlinear robust optimization using the affine decision rule was evaluated successfully, on a simple case study, as well as a larger, practical example.

## 6.2 Future work

Based on the work done in this thesis, the following potential avenues have been identified, for future work.

**Dealing with multiple sources of uncertainty**

In this thesis, only a single source of primitive uncertainty $\xi$ was considered - in the case of the small water treatment model, the primitive uncertainty affected source flow $F_s(\xi)$, and in the case of the SAGD model, it affected the steam demand from the reservoir $Demand^{steam}(\xi)$. In practice, however, uncertainty in the model is expected to arise from additional sources such as contaminant concentration, treatment unit removal efficiency, and other such parameters. The application of the proposed methods in the thesis to a model affected by multiple sources of uncertainty could be a potential future work.

**Dealing with uncorrelated uncertainty**

In this thesis, all the source flows in the small water treatment model were assumed to be affected by the same primitive uncertainty $\xi$, thus giving rise to correlation. Potential future work can be done to assess the application of the methods developed in this thesis for uncorrelated source flows, to analyze the changes in the solution.

**Different formulations of the uncertainty set**

In this thesis, the uncertainty set was defined using lower and upper bounds, as described in Section 1.6.4. The application of the methods developed in this thesis to other uncertainty set formulations such as box sets, ellipsoidal sets, etc. can be evaluated in the future. Another avenue of interest is the use of data-driven optimization - this class of optimization leverages machine learning techniques using process data, to obtain information about the uncertainty set probability distribution.

**Developing an algorithm for global optimum search**

In this thesis, all the decision rules obtained through the solution of the stochastic LDR formulations of small water treatment model as well as the SAGD model pertained to the local optimal solution. In the future, an algorithm for the global optimum search can be developed.

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