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Thesis for Ph. D. degree

Development of Simulation-Optimization Models for Agricultural Contaminant Loading Management Considering Effects of Groundwater Pumping

Park, Dong Kyu

August 2014

School of Earth and Environmental Sciences Seoul National University
Development of Simulation-Optimization Models
for Agricultural Contaminant Loading Management
Considering Effects of Groundwater Pumping

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A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Earth and Environmental Sciences

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School of Earth and Environmental Sciences
Seoul National University
ABSTRACT

In agricultural regions, a significant amount of groundwater has been used but agricultural activities, such as greenhouse farming, have often threatened its quality. Therefore, it is necessary to suitably manage the agricultural contaminant loading for sustainable groundwater use in those regions. However, pumping condition should also be considered in the management because groundwater pumping can change the fate of contaminant in the subsurface such as its leaching to the water table and migration in the aquifer. In this study, based on the field investigation and monitoring, an agricultural contaminant loading management model was developed in order to determine the optimal permissible contaminant loading mass for a given pumping condition, using simulation-optimization method. Periodical on-ground contaminant loading on non-point sources such as fertilizer application in greenhouse was simulated by integrating the 1-D analytical solution for solute transport in the unsaturated zone and the 3-D numerical model for groundwater flow and solute transport in the saturated zone. Backward transport simulation was applied to the model in order to evaluate the relative importance of contaminant sources quantitatively. Genetic algorithm was linked to this integrated simulation
model as optimization technique. This model could be useful in the agricultural contaminant loading management in the agricultural regions where many potential non-point sources were located at. Using this model, the optimal contaminant loading designs obtained under various pumping conditions were compared in order to examine the effects of pumping conditions in determining the optimal contaminant loading. The results demonstrated that the optimal contaminant loading designs were determined differently according to the given pumping conditions. Another management model was developed to manage permissible on-ground contaminant loading mass and pumping rates simultaneously. This model cannot consider only dynamics between fate of contaminant and pumping but also various conditions such as different usage of, or demand on, each pumping well and contaminant source in a single of optimization process. The optimal design determined from this model allowed more amounts of both of contaminant loading and groundwater pumping than any other optimal design suggested previously. In addition, in the agricultural regions where groundwater has been used intensively in a specific period of time, such as rice-growing season, it must be particularly important to consider such pumping condition in the agricultural contaminant management. Therefore, the model to simultaneously manage agricultural contaminant loading and groundwater
use under time-variant pumping condition was also developed. For this, the method to approximate the contaminant leaching to the fluctuating water table caused by a regular schedule of groundwater pumping was suggested and transient groundwater flow simulation was applied. In the optimal design obtained under the time-variant pumping condition, the contaminant loading was restricted considerably because a relatively large amount of contaminant leaching to the shallow depth of water table during the period without groundwater pumping, a strong inflow of contaminant to the wells driven by the large amount of pumping during the period with groundwater pumping, and a sudden increase of contaminant leaching immediately after stopping the operation of pumping. Particularly, the optimal design obtained under the no-pumping condition in this study was to imitate some previous studies about agricultural contaminant management which had not considered any pumping condition, in order to demonstrate the importance of considering pumping condition in the agricultural contaminant loading. The result showed that the agricultural contaminant loading management without considering pumping condition could fail in the regions where groundwater use has been common.

Keywords : Agricultural contaminant loading management; Nitrate;
Fertilizer application in greenhouse; Simulation-optimization model; Groundwater pumping; Water table fluctuation; Permissible on-ground loading mass.
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CHAPTER I. INTRODUCTION

1. Backgrounds of this study

In many agricultural regions both agriculture and municipal water users rely heavily, or often exclusively, on clean, reliable sources of groundwater. However, certain agricultural activities have sometimes had detrimental effects on the environment as results of groundwater contamination (Spalding and Exner, 1993; Wang et al., 1996; Skinner et al., 1997; Roseta-Palma, 2003; Chae et al., 2004; Almasri and Kaluarachchi, 2007; Masetti et al., 2008; Jiang and Somers, 2009; Peña-Haro et al., 2009, 2010; Wei et al., 2009, Park et al., 2014). In particular, the excessive use of nitrogen-based fertilizer and manure often results in nitrate contamination to the groundwater, which may be harmful to human health, damage crop productivity, and lead to eutrophication of surface water (Newbould, 1989; Lee et al., 1991; Spalding and Exner, 1993; Taghavi et al., 1994; Hayashi and Rosenberry, 2002; Chae et al., 2004; Almasri and Kaluarachchi, 2005a; Peña-Haro et al., 2009; Wick et al., 2012). The deterioration of agricultural groundwater quality can affect the sustainability of groundwater use,
limiting the supply of available water and imposing remediation costs (Peña-Haro et al., 2009). Nevertheless, these activities cannot arbitrarily be restricted for only the groundwater quality protection and thus it is necessary to find a way to manage the activities which can prevent groundwater contamination as well as guarantee agricultural productivity (Almasri and Kaluarachchi, 2004a, 2005a; Park et al., 2014).

Several integrated approaches for agricultural contaminant loading management have been explored in order to incorporate hydrological, environmental, and economic considerations in estimating nitrate leaching and determining appropriate on-ground fertilizer application (Shaffer et al., 1991; Almasri and Kaluarachchi, 2005a,b; Peña-Haro et al., 2009, 2010; Wei et al., 2009). However, these studies did not take into account any potential influences of groundwater pumping, even though groundwater has been used commonly in many agricultural regions. Generally, groundwater pumping lowers the water table and distorts groundwater flow. Consequently, it could have significant impacts on the fate of contaminants in the subsurface, such as its leaching to the water table and migration in the aquifer (Willis and Yeh, 1987; Taghavi et al., 1994; Almasri and Kaluarachchi, 2004a). Eventually, the effects of groundwater pumping will have a decisive influence even on the contaminant loading management. A
few studies have given comprehensive insights into managing groundwater quantity and quality together economically (Roseta-Palma, 2002, 2003) and hydrologically (Gharbi and Peralta, 1994; Keshari and Datta, 1996). In particular, Roseta-Palma (2002, 2003) pointed out that many agricultural regions have had a problem for both of groundwater quantity and quality at the same time and emphasized the importance of this integrated management, indicating that the value of water depended on the quantity of water available based on its quality. However, the former studies were based solely on the economic values of groundwater quantity and quality, without considering the physical processes of groundwater flow and solute transport, and the latter studies focused on the indirect management of groundwater quality, by controlling pumping rates and/or scheduling, rather than contaminant loading from on-ground sources. In a broad sense, many studies about groundwater quality management might also belong to the latter. For example, they determined the optimal pumping control to remove the contaminant plume (e.g., Ko et al., 2005) or to prevent the saltwater intrusion (e.g., Park and Aral, 2004). The unexceptional fact that pumping can spread or shrink a contaminant plume, which these studies were based on, must be another reason that groundwater quantity should be considered in its quality management and it is necessary to manage the both together.
In agricultural regions where groundwater use has been concentrated in a specific period of time, it is particularly important to consider pumping conditions in managing contaminant loading. For example, rice farming requires a significant amount of water during the growing season, and most or a large portion of the required water has often come from groundwater because of its spatial proximity and availability. As a result, groundwater level and flow field in those regions tend to change from season to season, and so does the fate of contaminant. This indicates that contaminant loading management in those regions should be performed with consideration of the fate of contaminants under time-variant pumping condition.

2. Objectives of this study

The main objectives of this study were to demonstrate the effects and importance of considering the existing groundwater pumping conditions on agricultural contaminant loading management, and to develop contaminant loading management models more appropriate and practical for agricultural regions where groundwater has been commonly used. First of all, several times of field investigations and monitoring were carried out to understand groundwater use and quality in an agricultural region located in Icheon,
Korea, in 2008 and 2009 (Chapter II). Based on these investigations, a management model to determine the optimal permissible periodical on-ground loading mass was developed using simulation-optimization method (Chapter III). An analytical solution for solute transport in the unsaturated zone was integrated with a 3-D groundwater flow and solute transport model. Genetic algorithm was linked with this integrated simulation model and backward transport simulation was also considered to evaluate each relative importance of contaminant sources. Numerical experiments were performed to evaluate effects of pumping condition on the optimal contaminant loading designs (Chapter IV). The optimal contaminant loading designs obtained under various pumping conditions were compared each other and another management model was developed to optimize both the permissible on-ground contaminant loading mass and the pumping rates simultaneously. Finally, the management model was expanded to manage agricultural contaminant loading in regions where a significant amount of groundwater extraction is concentrated in a specific period of time (Chapter V). A method to approximate contaminant leaching to a fluctuating water table and the transient-flow simulation were suggested to simulate the fate of contaminants under time-variant pumping conditions (Park et al., 2014).
CHAPTER II. SITE DESCRIPTION AND FIELD INVESTIGATION

1. Site description

Field investigation and monitoring of agricultural groundwater use and nitrate contamination were carried out in an agricultural field of about 2 km\(^2\) located at the northeastern in Icheon, Korea (Figure II-1). Geologically, this study area is dominated by Jurassic biotite granite on the low altitude of mountain below EL. 100 m and Quaternary alluvium distributed along the Bokha stream (Geological and Mineral Institute of Korea, 1975/Figure II-2). Although the greenhouse area has been expanding, occupying fields that were previously rice paddies, the majority of the study area remains covered by rice paddies. In the study area, which requires a significant amount of water supply during every rice-growing season, groundwater is the main water supply, despite concerns of a groundwater shortage caused by over-extraction. The aerial photographs taken by Korea Forest Research Institute (http://aerophoto.kfri.go.kr), Icheon GIS service (http://gis.icheon.go.kr), and Daum Skyview (http://map.daum.net) over the years, 2004–2009,
showed an increase of greenhouse facilities in this study area (Figure II-3). For example, during this period, the number of greenhouses increased from 161 to 304 and the area of greenhouses increased approximately from 12 ha to 22ha. This recent increase of greenhouse facilities could be a threat to the groundwater quality in the study area because vegetables, fruits, and flowers that are mainly grown in the greenhouses have usually required an amount of nitrogen-based fertilizer (Ritter and Shirmohammadi, 2001). In addition, fertilizers must be applied more frequently in the greenhouse than in the rice paddy because crop cultivation and harvest in greenhouses can proceed all the year round with little concerns for weather. The well-drained soil in the greenhouse may also facilitate the leaching of fertilizer constituents, such as nitrate, onto aquifer (Almasri, 2007; Hajhamad and Almasri, 2009).
Figure II-1. Map of the study area
Figure II-2. Geological map of the study area
Figure II-3. Increase of greenhouse facilities in the study area, from 2004 to 2009
2. Field investigation and monitoring in the study area

In the study area, most agricultural groundwater wells located near rice paddies and greenhouses were installed within 10m depth from the ground surface. Redox potential and dissolved oxygen measured in these wells were in the range of 200–300 mV and 5–6 mg/L, respectively. Thus, the aquifer is under oxidizing and aerobic conditions, implying that nitrate leached from a nitrogen-based fertilizer would be transported with groundwater flow, without undergoing active mass reduction by denitrification (Tesoriero et al., 2000; Almasri and Kaluarachchi, 2004a; Chae et al., 2004). Nitrate concentrations measured in these wells were mostly above 3 mg NO3-N/L (Figure II-4(a)).

Agricultural wells such as NSY1, SY1, NSY2, SY5, BW5, WG5, and WG3, which are located inside or nearby greenhouses, showed extreme fluctuations of nitrate concentrations over time (Figure II-4(b)). The peak concentrations were sometimes above the drinking water standard. This somewhat irregular pattern might result from a complex interaction of periodical fertilizer application, soil nitrogen cycle, soil and aquifer characteristics, individual farming method and schedule, groundwater pumping, seasonal precipitation, and so on (Almasri and Kaluarachchi,
2004a, b; Masetti et al., 2008; Wick et al., 2012). Actually, the effects of all these factors on those wells must be very difficult to be characterized and quantified accurately (Tesoriero and Voss, 1997; Almasri and Kaluarachchi, 2004a,b, 2005a,b), particularly in the study area where most of the greenhouse farming has been small-scale and individual. However, in the study area where $2.772 \times 10^6$ m$^3$/year of groundwater use for agriculture and more than 100 pumping wells for rice-farming were reported (KORMAF and KRC, 2006), the extensive groundwater pumping for large-scale rice farming might especially affect the fate of agricultural contaminants loaded from the greenhouses. In contrast, nitrate concentrations measured in the agricultural wells near rice paddies and the domestic wells for residents were steadier with lower values than the wells near the greenhouses (Figure II-4(a)). The impermeable or low-permeable soil layer formed on the rice paddies appears to be preventing or minimizing nitrate leaching (Nolan et al., 2002; Almasri and Kaluarachchi, 2005b). All domestic wells were installed at depths of more than 30 m. The low nitrate concentrations in the deep well can be explained to be relatively slow vertical movement in the aquifer (Hallberg, 1989) and denitrification in reducing condition (Spalding and Exner, 1993).

The major cations and anions in the groundwater sampled in June and
September 2008 was plotted for the use of wells in the piper diagrams (Figure II-5). The groundwater sampled in the wells for rice farming and domestic use was a Ca-HCO$_3$ type which was typical of shallow and fresh groundwater. However, the samples in the wells for greenhouse farming were a mixed cation-mixed anion type water, which had more Cl$^-$ and less HCO$_3^-$ than the wells for rice farming and domestic use. These changes may result from the agricultural activities in the greenhouse, such as fertilizer application and liming (Rajmohan and Elango, 2006). In September, in most of the wells Na$^+$ and K$^+$ were increased but Mg$^{2+}$ was decreased while any changes in anions was not shown.

In 2008–2009, hydraulic head was continuously monitored in NWG2 for greenhouse farming and public use, which was the only well allowing its monitoring in the study area (Figure II-6). Even although any decline in hydraulic head was actually not found during rice-growing season, maybe because of a large amount of precipitation in that time, the decrease in hydraulic head monitored in winter indicated intensive greenhouse farming and the resulting groundwater use during the winter. The groundwater pumping in NWG2 must significantly affect the fate in the subsurface zone of the fertilizers applied on the greenhouses during that time.

The kind and growth status of crops grown in the greenhouses were
investigated together with the kind of fertilizers in the study area. Various kinds of crops were grown on the greenhouses as shown in Table II-1, while lettuce was a main crop grown in these greenhouses. As well, although the same crop was grown in some greenhouses, a variety of growth statuses, from seeding to harvest, of the crop were found in each greenhouse on the same day. Various kinds of fertilizers were also found around the greenhouses, which were mainly composite, organic, ammonium, and urea types of fertilizers. In the study area, particularly, the fertilizer applications have been determined by an individual farming method and schedule of each farmer. Therefore, these results demonstrated that it is not easy to generalize and consider all of them in the development and application of model for contaminant loading management.
Figure II-4. NO₃-N concentrations measured in the wells
Figure II-5. Piper diagrams plotted according to the use of wells
Figure II-6. Hydraulic head measured in NWG2 in winter 2008–2010
<table>
<thead>
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<th>Crops</th>
<th>Wells</th>
<th>Crops</th>
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<td>NWG1</td>
<td>Leek</td>
</tr>
<tr>
<td>NSY1</td>
<td>Flower</td>
<td>WG2</td>
<td>Lettuce</td>
</tr>
<tr>
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<td>Lettuce</td>
<td>NWG2, NWG3</td>
<td>Lettuce, Spinach, Crown daisy, Leek</td>
</tr>
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<td>Lettuce</td>
<td>WG3</td>
<td>Lettuce</td>
</tr>
<tr>
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<td>Sedum</td>
<td>WG5</td>
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</tr>
<tr>
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<tr>
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<td>Guava, Strawberry</td>
<td></td>
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<tr>
<td>SY6</td>
<td>Leek</td>
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</tbody>
</table>
CHAPTER III. MODEL DEVELOPMENT FOR AGRICULTURAL CONTAMINANT LOADING MANAGEMENT

1. Introduction

The fertilizer applications in agricultural regions have a trade-off between agricultural income and groundwater quality. For example, the sufficient amount of fertilizer use may enhance crop growth and productivity but its excessive use can sometimes cause nitrate contamination of groundwater (Almasri and Kaluarachchi, 2004a). Therefore, it is necessary to develop the agricultural contaminant loading management model to determine the sustainable fertilizer application to satisfy the both demands for agricultural income and groundwater quality to acceptable levels. The changing concentrations of nitrate observed in only the wells located near greenhouse, shown in the Chapter II, might be evidence that the greenhouses have been non-point contaminant sources in this study area. Fertilizers in the greenhouses are applied periodically, according to the kind of crop, crop growth status, seeding and harvest, and so on, because crops
can generally be grown and harvested in there in all the year. Therefore, the management model has to be able to simulate the periodical on-ground contaminant loading, like the fertilizer applications in greenhouse.

Not all the contaminant sources distributed in a region may significantly cause a contamination to the wells because migration of contaminant plume is highly dependent on groundwater flow (Liu et al., 2005; Almasri, 2007). Therefore, the regulation in a lump over all the sources must be an overregulation for some sources that hardly affect the wells. The presence of these sources can also cause a problem in the optimization process if the objective function is simply formulated for the maximization of contaminant loading mass. For example, the optimal contaminant loading mass designed on such sources are likely to be always close to the maximum because contaminant loading on them would not increase concentration on the wells. As a result, the overall optimization process will be greatly dependent on the determination of contaminant loading only on these sources having a relatively large of fitness value, while the determinations of contaminant loading on the sources influential to wells are rather insignificant although more careful managements are actually needed. Thus, it is necessary to sort out the contaminant sources influential to the wells and to reflect them on the optimization process. The
well vulnerability analysis suggested by Frind et al. (2006) might have a
cue to the qualitative sorting of contaminant sources. The well vulnerability
was defined as how vulnerable a well is to the contamination from the
unknown/known sources. For its evaluation, they used the backward
transport simulation describing when and how much the contamination
detected in well had been originated from the possible contaminant sources
located in a site (Neupauer and Wilson 1999, 2001; Frind et al., 2006; Lim,
2009). Actually, it might also address when and how much those
contaminant sources will contribute to the contamination of well. In other
words, their approach could be useful in calculating the possible
contamination contributions to the well and the corresponding relative
importance of sources.

With all of these considerations, a simulation-optimization model for
agricultural contaminant loading management was developed in this study.
The simulation models for the solute transport in unsaturated zone and the
groundwater flow and solute transport in saturated zone were integrated in
order to simulate the fate of a solute that is loaded periodically on ground
surface, moves downward and leaches onto water table, and then moves
along groundwater flow. The optimization technique, genetic algorithm, was
linked with the integrated simulation model to obtain to find the optimal
permissible on-ground contaminant loading mass. In addition, the backward transport simulation procedure was added to the management model for agricultural contaminant loading in order to sort out the contaminant sources and to manage the influential sources significantly.

2. Methodology

2.1. Simulation-optimization model

The management model was developed using a simulation-optimization method based on the performed field investigation and monitoring, previously introduced in the Chapter II. To simulate the fate of contaminant loaded from on-ground sources, an analytical solution to approximate the solute transport in the unsaturated zone was integrated with a 3-D groundwater flow and solute transport model (Figure III-1). As an optimization technique, genetic algorithm was linked with the integrated simulation model. The objective function was established to allow for more contaminant loading. The overall optimization process for the developed model follows the flow chart shown in Figure III-2.
Figure III-1. Schematic illustration of the integrated simulation procedure
24

Figure III-2. Flow chart of the management process in this developed model
2.1.1. Integrated simulation model

2.1.1.1. Analytical solution for approximation of contaminant leaching mass

Equations for on-ground contaminant loading such as instantaneous fertilizer application in the greenhouses can be established as follows:

\[ C(x, 0) = C_i \] (III-1)
\[ C(0, t) = \begin{cases} C_0 & 0 < t \leq t_0 \\ 0 & t > t_0 \end{cases} \] (III-2)
\[ \frac{\partial C}{\partial x}(\infty, t) = 0 \] (III-3)

Assuming constant moisture content and fluid velocity, an analytical solution of solute transport subject to the above equations is given by (van Genuchten, 1981)

\[ C(x, t) = \begin{cases} (C_0 - \gamma / \mu)H(x, t) + L(x, t) & 0 < t \leq t_0 \\ (C_0 - \gamma / \mu) H(x, t) + L(x, t) - C_0 H(x, t - t_0) & t \geq t_0 \end{cases} \] (III-4)

where
\[ H(x,t) = \frac{1}{2} \exp \left[ \frac{(v-u)x}{2D} \right] \text{erfc} \left[ \frac{Rx - ut}{2(DRt)^{1/2}} \right] + \frac{1}{2} \exp \left[ \frac{(v+u)x}{2D} \right] \text{erfc} \left[ \frac{Rx + ut}{2(DRt)^{1/2}} \right] \]

(III-5)

\[ L(x,t) = \left( \frac{\gamma}{\mu} - C_i \right) \exp \left( -\frac{\mu t}{R} \right) \left\{ \frac{1}{2} \exp \left( \frac{Rx - vt}{2(DRt)^{1/2}} \right) + \frac{1}{2} \exp \left( \frac{vx}{D} \right) \text{erfc} \left[ \frac{Rx + vt}{2(DRt)^{1/2}} \right] \right\} + \frac{\gamma}{\mu} + \left( C_i - \frac{\gamma}{\mu} \right) \exp \left( -\frac{\mu t}{R} \right) \]

\[ u = v(1 + 4 \mu D / v^2)^{1/2} \]  

(III-6)

(III-7)

where \( C(x, t) \) is the concentration at depth \( x \) and time \( t \) [ML\(^{-3}\)]; \( C_0 \) is the loading concentration of the solute [ML\(^{-3}\)]; \( C_i \) is the initial background concentration [ML\(^{-3}\)]; \( \gamma \) is the zero-order source term [ML\(^{-1}\)T\(^{-1}\)]; \( \mu \) is the first-order decay rate [T\(^{-1}\)]; \( t_0 \) is the solute loading time on the source [T]; \( v \) is the pore water velocity [LT\(^{-1}\)]; \( R \) is the retardation factor [-]; and \( D \) is the dispersion coefficient [L\(^2\)T\(^{-1}\)].

This analytical solution describes vertical transport of a solute of initial concentration \( C_0 \) loaded at the top boundary at loading time \( t_0 \).

Breakthrough curves describing that the pulse-type contaminant loading undergoes advection and dispersion in the unsaturated zone can be obtained from this solution. The calculated concentrations are converted to the mass in a certain volume of water with a vertical flow related to irrigation under
the assumption that contaminant totally dissolves to groundwater as soon as it reaches water table and then are used as an input for the source term in the saturated solute transport model. In order to simulate the periodical fertilizer applications, which is repeated in greenhouses every few months, the breakthrough curves obtained from each single loading event are superposed according to their loading period (Figure III-3). If the contaminant from the previous loading did not completely leach to the water table until the next loading, the remaining mass is added to the leaching mass from the next loading event. For this, a single of breakthrough curve is calculated for a double of loading period of each contaminant source.
\[ M_i : \text{Leaching mass at } i\text{-th time step} \]
\[ (M_i = MS_{(i,j)} + MR_{(i, j-1)}) \]

**MS_{(i,j)}**: Mass at the \(i\)-th time step from the \(j\)-th loading event

**MR_{(i, j-1)}**: Remaining mass at \(i\)-th time step from \(j-1\)-th loading event

**Breakthrough curve derived for the total simulation time**

**Loading period**

**Calculation time for breakthrough curve from a single loading event**
\[ = \text{Loading period} \times 2 \]

**Figure III-3.** Calculation of leaching mass from periodical contaminant loading using superposition of breakthrough curves
2.1.1.2. Groundwater flow and solute transport in the saturated zone

Groundwater flow and solute transport are governed by the following partial differential equations, respectively:

\[
S_s \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + q_s \quad \text{(III-8)}
\]

\[
R \frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) - \nabla \cdot (v C) + \frac{q_s}{\theta} C_s + \left( \frac{\partial C}{\partial t} \right)_{\text{rxn}} \quad \text{(III-9)}
\]

where \( S_s \) is the specific storage \([L^{-1}]\); \( t \) is the time \([T]\); \( h \) is the hydraulic head \([L]\); \( K \) is the hydraulic conductivity tensor \([LT^{-1}]\); \( q_s \) is the source/sink term \([T^{-1}]\); \( R \) is the retardation factor \([-]\); \( C \) is the solute concentration \([ML^{-3}]\); \( D \) is the hydrodynamic dispersion tensor \([L^2T^{-1}]\); \( v \) is the average linear velocity \([LT^{-1}]\); \( \theta \) is the porosity \([-]\); \( C_s \) is the concentration of the source/sink flux \([ML^{-3}]\); and \( \left( \frac{\partial C}{\partial t} \right)_{\text{rxn}} \) is the biological/chemical reaction term. The depth to the water table is used to calculate the leaching mass in the unsaturated model. In this study, Hydrogeosphere (Therrien et al., 2010) was used to simulate 3-D groundwater flow and solute transport.
2.1.2. Optimization model

Genetic algorithm searches for the global optimum using three basic operators, namely reproduction, crossover, and mutation, based on the evolution mechanisms of natural genetics and survival of the fittest (Goldberg, 1989; Ko et al., 2005/Figure III-4), and it has widely been used in water resources management (Nicklow et al., 2010). The genetic algorithm was linked with the integrated simulation model introduced previously. With the weighted sum method, an objective function was formulated to maximize the permissible on-ground contaminant loading mass, subject to constraints for concentration. In other words, it was to minimize the limitation of fertilizer application in greenhouses and to prevent well contamination, as follows:

Maximize $fit_{total} = \left( \frac{\sum M_{GH}}{c_p \cdot P} \right)$ (III-10)

subject to

$$P = \left[ \max \left( 0, \frac{C_{AW}^{\text{max}} - C_{AW}^*}{\alpha_{AWC}} \right) \right]^n + \left[ \max \left( 0, \frac{C_{DW}^{\text{max}} - C_{DW}^*}{\alpha_{DWC}} \right) \right]^n + \beta$$ (III-11)
with constraints \( C_{AW}^{\text{max}} < C_{AW}^* \); \( C_{DW}^{\text{max}} < C_{DW}^* \); and \( M_{GH} \leq M^* \) (III-12)

where \( \text{fit}_{\text{total}} \) is the total fitness value [-]; \( P \) is the penalty value [-]; \( M_{GH} \) is the permissible on-ground contaminant loading mass for each greenhouse group [M]; \( c_p \) is the cost coefficient for the penalty [-]; \( C_{AW}^{\text{max}} \) and \( C_{DW}^{\text{max}} \) are the maximum concentrations in wells for agricultural use, located by rice paddies and greenhouses, and domestic wells, respectively [ML\(^{-3}\)]; \( C_{AW}^* \) and \( C_{DW}^* \) are the concentration constraints for agricultural and domestic use, respectively [ML\(^{-3}\)]; \( \alpha_{AWC} \) and \( \alpha_{DWC} \) are the violation allowances for the concentrations in agricultural and domestic wells, respectively [-]; \( n \) is the coefficient for magnifying each penalty value exponentially [-]; \( \beta \) is a constant to ensure that the denominator of the objective function is non-zero [-]; and \( M^* \) is the loading mass constraint [M].
<table>
<thead>
<tr>
<th>Gene</th>
<th>Binary Code</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Gene 1" /></td>
<td><img src="image2" alt="Binary Code 1" /></td>
</tr>
<tr>
<td><img src="image1" alt="Gene 2" /></td>
<td><img src="image2" alt="Binary Code 2" /></td>
</tr>
<tr>
<td><img src="image1" alt="Gene 3" /></td>
<td><img src="image2" alt="Binary Code 3" /></td>
</tr>
</tbody>
</table>

**Selection**
- ![Selection](image1)
- Binary Code: 101010
- 010101

**Crossover**
- ![Crossover Site](image1)
- ![Crossover](image1)
- Binary Code: 101010
- 010101

**Mutation**
- ![Mutation](image1)
- Binary Code: 101010
- 010101

---

**Figure III-4.** Three operators of genetic algorithm (Ko et al., 2005)
Based on the fact that agricultural income is primarily associated with crop yield and the assumption that the crop yield is proportional to only the fertilizer mass applied within its maximum, the loading mass term in the objective function, $M_{GH}$, can be substituted into the sum of the revenue expected from the fertilizer application in each greenhouse group, as a contaminant source, $RV_{GH}$, with the following equation:

$$RV_{GH} = P_{GH} \cdot \frac{Y_{GH}^{\text{max}}}{M_{GH}^{\text{max}}} \cdot M_{GH} \cdot A_{GH} \cdot f_{GH} \quad \text{(III-13)}$$

where $RV_{GH}$ is the total expected revenue at each greenhouse group within the entire period; $P_{GH}$ is the price of the crop grown in each greenhouse group; $M_{GH}^{\text{max}}$ is the maximum permissible fertilizer application mass per unit area in each greenhouse group; $Y_{GH}^{\text{max}}$ is the maximum crop yield per unit area expected from the fertilizer application of $M_{GH}^{\text{max}}$ in each greenhouse group; $M_{GH}$ is the loading mass per unit area designed for each greenhouse group; $A_{GH}$ is the area of each greenhouse group; and $f_{GH}$ is the fertilization frequency for each greenhouse group in the entire period. The product of the second, third, and fourth terms is the crop yield expected from the fertilizer application of $M_{GH}$ in each greenhouse group having the
area of $A_{GH}$, which is then multiplied with the first term to calculate the revenue expected from a single harvesting. Because fertilizer and manure are generally applied to enrich soil again after harvesting and before seeding, the fertilization frequency can be regarded as the number of crop harvests. Thus, by multiplying the product with the fifth term, the total revenue expected from the entire harvest in each greenhouse group during the entire period, $RV_{GH}$, was calculated.

2.1.3. Backward transport simulation for relative importance of contaminant sources

The well vulnerability analysis suggested by Frind et al. (2006) can give a hint to qualitatively evaluate the relative importance among contaminant sources and to sort out the influential sources. They assessed the well vulnerability addressing the potential impact of contaminant sources within a capture zone with the backward transport simulation. The backward transport modeling generally provides information about prior locations and transport history of a contamination detected in well with one simulation run (Neupauer and Wilson 1999, 2001; Frind et al., 2006). It can be used to improve characterization of known sources of groundwater.
contamination, to identify previously unknown contaminant sources, to
delineate capture zone, and so on.

Neupauer and Wilson (1999, 2001) suggested that the backward
transport equation can be derived from the general advection-dispersion
equation using the adjoint method. The adjoint equation for backward solute
transport was given by

\[ R \frac{\partial \psi^*}{\partial \tau} = \nabla \cdot (D \nabla \psi^*) + \nabla \cdot (v \psi^*) + \frac{q_s}{\theta} \psi^* + \left( \frac{\partial \psi^*}{\partial \tau} \right)_{ran} \]  (III-14)

\[ \psi^*(x_0, \tau; x_w) = \frac{dC(x_w, t)}{dM_0(x_0)} \]  (III-15)

where \( \psi^* \) is an adjoint state of the original variable \( C \) [L\(^{-3}\)]; \( \tau \) is the backward
time that is time prior to a certain time of interest [T]; \( x_0 \) is the source
location; \( x_w \) is the well location; \( M_0(x) \) is the initial solute mass at location \( x \).
Given the forward transport equation, the backward transport equation can
be technically obtained by reversing the sign of flow field and by adapting
the boundary conditions (Neupauer and Wilson, 1999, 2001; Lim, 2009/
Figure III-5). The details of this method were presented in Neupauer and
(a) general (forward) solute transport

(b) backward solute transport

Figure III-5. Schematic illustration showing the processes of simulating solute transport from many possible sources to a well (Lim, 2009)
The backward travel-time probability describes the amount of time required for a solute to travel to the sampling location from some upgradient location (Newpauer and Wilson, 2001; Lim, 2009) and was given by

\[ p_t(t;x_w,x_0) = \theta(x_w)\nu(x_w,t)|A(x_w)\psi^*_\tau(x_0,\tau;x_w) \quad (III-16) \]

\[ \psi^*_\tau(x_0,\tau;x_w) = \frac{dC^f(x_w,t)}{dM_0(x_0)} \quad (III-17) \]

where \( p_t(t;x_w,x_0) \) is the backward travel-time probability of a solute traveling to the pumping well at \( x_w \) from an upgradient location \( x_0 \) \([T^{-1}]\); \( \theta(x) \) is the porosity at location \( x \) [-]; \( \nu(x) \) is the local average linear velocity at location \( x \) \([LT^{-1}]\); \( A(x) \) is the area orthogonal to flow at location \( x \) \([L^2]\); \( \psi^*_\tau \) is an adjoint state of the flux concentration \( C^f \) \([L^{-3}]\). Hydrogeosphere (Therrien et al., 2010), introduced in the previous chapter, can also simulate backward solute transport and, as a result, obtain backward travel-time probability.

Because many contaminant sources in the agricultural regions, such as greenhouses, are non-point sources, it is necessary to define the backward travel-time probability for those sources. Lim (2009) suggested the backward travel-time probability for the non-point contaminant source as areal-average of travel-time probabilities calculated on each node.
corresponding to the sources and it was given by

\[ p_t (t; x_w, X_0) = \theta(x_w) |v(x_w, t)| A(x_w) \psi^*_x (X_0, \tau; x_w) \] (III-18)

\[ \psi^*_x (X_0, \tau; x_w) = \frac{1}{X_0} \int_{X_0} \psi^*_x (x_{0i}, \tau; x_w) d\Omega, \quad x_{0i} \in X_0 \] (III-19)

where \( X_0 \) is the area of non-point source [L^2]; \( x_{0i} \) is the area of each node in the source [L^2]; \( \Omega \) is the space where the probabilities are evaluated. In addition, Lim (2009) defined the backward travel-time probability for multiple wells and non-point sources by normalizing each probability for each well by the number of wells and it was given by

\[ p_t (t; X_w, x_0) = \frac{1}{N} \sum_{i=1}^{N} p_t (t; x_{wi}, x_0), \quad x_{wi} \in X_w \] (III-20)

Frind et al. (2006) demonstrated that with a scale factor the breakthrough curves for concentration from a contaminant source to a well can be identical to the curves of travel-time probability from the well to the source. Particularly, the dimension of concentration normalized by loading mass in forward simulation, \( C/M_0 [ML^{-3}/M=\text{L}^{-3}] \), is compatible with that of
time-travel probability normalized by pumping rates in backward transport, $P_t/q [T^{-1}/L^3T^{-1}]=L^{-3}$], while the scale factor is dimensionless and unique for the given groundwater flow system (Frind et al., 2006). In other words, the scaled backward travel-time probability can be equivalent to the concentration and Lim (2009) defined it as expected concentration $C_E$.

$$C_E = \frac{M_0 \cdot S_f}{q} \cdot p_t \quad \text{(III-21)}$$

where $q$ is the pumping rates [$M^3T^{-1}$]; $S_f$ is the scale factor [-]. However, under a given pumping condition, pumping rate and scale factor are constant. Therefore, the backward probability scaled by only the loading mass $M_0$ can be regarded as an incomplete form of contaminant concentration from the source. The incomplete-scaled travel-time probability obtained under the given pumping condition is available to sort out the influential contaminant sources because the importance of sources will be evaluated relatively.

2.1.3.1. Application of backward transport simulation to the management model
The backward transport simulation was used to qualitatively address how vulnerable the well is to contamination from several possible sources in Frind et al. (2006), but it also can describe how much and what contaminant sources contributed to the detected well contamination because backward probability describes information for a detected contaminant to travel to the well from some upgradient locations. In this study, the contamination contributions of sources were estimated from the backward transport simulation in order to identify the relative importance of each source. If the forward transport simulation was used in order to identify the contaminant contribution of sources, one simulation must individually be run for each contaminant source. The potential exposure of well to contamination above a specific threshold was used as an index to quantify the contamination contribution of sources to a well for a single of contaminant loading. It was formulated with an integration of the incompletely scaled travel-time probabilities above a prespecified threshold over the corresponding exposure time (Figure III-6). The relative importance of source was defined as the ratio of the contamination contribution calculated for each source to the total contributions. The contaminant contribution and the relative importance of sources is given by
\[ C_{tr, GH} = \int_{t_L}^{t_E} p(t; x_w, X_{GH}) \cdot M_{GH} \, dt \quad \text{(III-22)} \]

\[ \omega_{GH} = \frac{C_{tr, GH}}{\sum C_{tr, GH}} \quad \text{(III-23)} \]

where \( C_{tr, GH} \) is the contamination contribution of each greenhouse group [M]; \( t_E \) is the time that the travel-time probability scaled by the loading mass from source to well is above a specified threshold [T]; \( \omega_{GH} \) is the relative importance for each greenhouse group [-].

Eventually, the relative importance of source was used as the weighting factor for the contaminant loading on each source in the objective function. The reformulated objective function is given by

\[ \text{Maximize} \quad fit_{total} = \left( \frac{\sum \omega_{GH} \cdot M_{GH}}{c_p \cdot P} \right) \quad \text{(III-24)} \]

The overall procedure of modified simulation-optimization model, adding the backward transport simulation procedure, was presented in

**Figure III-7.** A small value of relative importance of a source, or its contaminant contribution, implies that any regulation for groundwater quality protection will not be necessary on that source. Therefore, in this
model, if the relative importance of a contaminant source is small enough to ignore its impact, the maximum of contaminant loading will be assigned on the source. For a computational efficiency, in this procedure, the water table depth calculated in the backward transport simulation was used in estimating the leaching mass from on-ground contaminant loading.
Figure III-6. An example of calculating contaminant contribution of sources.
Figure III-7. Flow chart of the management process adding the backward transport simulation procedure
3. Results and discussion

3.1. Case study for application of backward transport simulation

3.1.1 Model domain and settings

A simple domain was presented to evaluate usefulness of the backward transport simulation procedure, added in order to obtain relative importance of contaminant source. The domain size was 350 m (width) × 340 m (length) × 30 m (thick) and was discretized into 34 rows, 35 columns, and 3 layers (Figure III-8). The assumed aquifer was homogeneous, having a hydraulic conductivity of $5.0 \times 10^{-4}$ cm/s. Constant head boundaries were assigned on the upper ($h_u = 28.0$ m) and the lower ($h_l = 25.0$ m) sides and no-flow boundaries were imposed on the left and the right sides. Therefore, the resulting groundwater flow direction was from the upper to the lower side. Initial concentrations over the entire domain and constant concentration boundary at the upper side were set to be 3 mg/L as the background concentration. The well PW1 having a pump at 20 m depth was located at the center of domain. The pumping rate was 85.3 m$^3$/day and the resulting drawdown was calculated to 6.97 m at the PW1. The periodical on-
ground contaminant loading were assumed on five non-point sources having an area of 900 m² and a loading period of 180 days. The optimal on-ground contaminant loading mass on each source as a decision variable was determined in range of 0.1 to 20 kg/a. The simulation time for the optimization was 10 years. The concentration constraint was set to 10 mg/L. Details on the properties of the saturated and unsaturated zones were summarized in Table III-1.
\[ h_u = 28.0 \text{ m} \]
\[ h_l = 25.0 \text{ m} \]
\[ q_{PW} = 85.3 \text{ m}^3/\text{day} \]

**Figure III-8.** Model domain and settings assumed in the case study for application of backward transport simulation procedure
Table III-1. Material properties for (a) the unsaturated zone and (b) the saturated zone

(a) unsaturated zone

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pore water velocity (v)</td>
<td>$1.07 \times 10^{-4}$ cm/s</td>
</tr>
<tr>
<td>Dispersion coefficient (D)</td>
<td>$0.0465$ m$^2$/day</td>
</tr>
<tr>
<td>First-order decay rates ($\mu$)</td>
<td>$1.0 \times 10^{-11}$ day$^{-1}$ (for non-zero)</td>
</tr>
<tr>
<td>Retardation factor (R)</td>
<td>1.0</td>
</tr>
<tr>
<td>Zero-order source term ($\gamma$)</td>
<td>$0.0$ m/L/day</td>
</tr>
<tr>
<td>Loading time ($t_0$)</td>
<td>1 day</td>
</tr>
<tr>
<td>Initial concentration ($C_i$)</td>
<td>0.0 mg/L</td>
</tr>
</tbody>
</table>

(b) saturated zone

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic conductivity ($K$)</td>
<td>$5.0 \times 10^{-4}$ cm/s ($K_V = 0.1K_H$)</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.25</td>
</tr>
<tr>
<td>Dispersivity ($\alpha_L$, $\alpha_T$, $\alpha_V$)</td>
<td>$10.0$, $0.1$, $0.01$ m</td>
</tr>
<tr>
<td>Retardation factor (R)</td>
<td>1.0</td>
</tr>
<tr>
<td>First-order decay rates ($\mu$)</td>
<td>0.0 day$^{-1}$</td>
</tr>
</tbody>
</table>
3.1.2 Effects of the relative importance of source on the optimal contaminant loading design

For the given groundwater flow condition, the optimal contaminant loading designs with and without considering the relative importance of sources were compared (Table III-2). The optimal design considering the relative importance of sources suggested that the contaminant loading of 3.7 kg/a allowed on the source S3 having the relative importance of 0.26 [-], which was the most influential source on the contamination of PW1. For the S4 that was the second influential source, the contaminant loading of 6.4 kg/a was allowed. The result that more amount of contaminant loading on the S4 was allowed than the S3 might be reasonable because more influential source would impact more on well and thus have to be regulated more. In the other hand, the small value of relative importance on S2, 0.06 [-], indicated that this source is hardly relevant to the contamination of PW1. Even if more than 2.9 kg/a amount of contaminant was loaded on this source, it would have little influence on PW1.

In the other hand, the optimal design without considering the relative importance of sources suggested that the contaminant loading on S2 was allowed up to 15.6 kg/a. The fitness value of S2 accounted for 73% of the
total fitness value of this design. This result indicated that the optimal
design had been determined depending on the loading mass assigned on S2,
which had been the least influential source. On the other hand, only the
loading mass of 1.0 and 2.3 kg/a were allowed on S3 and S4, that had been
the most influential contaminant sources, respectively although more
amount of contaminant loading can been allowed as shown in the previous
design considering the relative importance. These results supported the
usefulness of the suggested backward transport simulation procedure in the
optimization for contaminant loading management, particularly under the
condition that several possible contaminant sources were distributed widely.
Table III-2. Optimization results obtained (a) with considering the relative importance of contaminant sources using backward transport simulation procedure and (b) without considering the relative importance of contaminant sources.

(a) with relative importance of contaminant sources

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
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<tbody>
<tr>
<td>Loading mass (kg)</td>
<td>22.8</td>
<td>26.3</td>
<td>33.2</td>
<td>57.4</td>
<td>9.0</td>
<td>9.0</td>
</tr>
<tr>
<td>M/A (kg/a)</td>
<td>2.5</td>
<td>2.9</td>
<td>3.7</td>
<td>6.4</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Relative importance (-)</td>
<td>0.14</td>
<td>0.06</td>
<td>0.26</td>
<td>0.24</td>
<td>0.19</td>
<td>0.11</td>
</tr>
<tr>
<td>Fitness value (-)</td>
<td>0.003</td>
<td>0.002</td>
<td>0.008</td>
<td>0.013</td>
<td>0.002</td>
<td>0.001</td>
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</tbody>
</table>

(b) without relative importance of contaminant sources

<table>
<thead>
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<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
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<tbody>
<tr>
<td>Loading mass (kg)</td>
<td>15.9</td>
<td>140.3</td>
<td>9.0</td>
<td>21.1</td>
<td>9.0</td>
<td>9.0</td>
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<tr>
<td>M/A (kg/a)</td>
<td>1.8</td>
<td>15.6</td>
<td>1.0</td>
<td>2.3</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Relative importance (-)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Fitness value (-)</td>
<td>0.002</td>
<td>0.022</td>
<td>0.001</td>
<td>0.003</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

1) Loading mass/Area
3.2. Optimal design result for agricultural contaminant loading

In order to examine effectiveness and applicability of the model developed in this study, a part of the study area in Icheon, Korea, where six groups of greenhouses had been located in 2009, was chosen as the model domain (Figure III-9). Most of the model settings followed the field investigation and monitoring introduced in Chapter II. This model domain and settings were also used to examine applicability of the management models developed in the next chapters.

3.2.1. Model domain and settings

The domain size was 490 m (width) \times 350 m (length) \times 50 m (thickness) and was discretized into 70 rows, 98 columns, and 5 layers. A coarse sand layer of 30 m thick was assumed to be underlain by a silty-sand layer of 20 m thick. Constant head boundaries were assigned on the left (48.0 m) and the right (46.5 m) sides and no-flow boundaries were imposed on the upper and the lower sides. Initial concentrations over the entire domain and constant concentration boundaries at the left and the right sides were set to be 3 mg/L as the background concentration. Because
groundwater has been used year-round for crops and residents in the
greenhouses in the study area, pumping rates of the agricultural wells for
greenhouse farming (GW) and the domestic wells for residents (DW) were
set to be kept at 10 and 5 m$^3$/day respectively in all the cases considering
groundwater pumping. The locations and number of wells and the areas and
locations of contaminant sources were determined based on the actual
situation investigated in the study area. Contaminants were assumed to be
periodically loaded on the on-ground non-point sources every four, five, and
six months, respectively, imitating greenhouse farming. Details on the
properties of the saturated and unsaturated zones and information on
contaminant sources and pumping wells were presented in Tables III-3 and
III-4, respectively. The concentration constraints were set to 20 mg/L for the
agricultural wells (GW and RW) and 10 mg/L for the domestic use well
(DWs) according to the Korean groundwater quality standard for
agricultural and drinking purposes for NO$_3$-N.
Figure III-9. Model domain for evaluating applicability of the models developed for agricultural contaminant loading management
Table III-3. Material properties for (a) the unsaturated zone and (b) the saturated zone

(a) unsaturated zone

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pore water velocity ($v$)</td>
<td>$1.07 \times 10^{-4}$ cm/s</td>
</tr>
<tr>
<td>Dispersion coefficient ($D$)</td>
<td>0.0465 m$^2$/day</td>
</tr>
<tr>
<td>First-order decay rates ($\mu$)</td>
<td>$1.0 \times 10^{-11}$ day$^{-1}$ (for non-zero)</td>
</tr>
<tr>
<td>Retardation factor ($R$)</td>
<td>1.0</td>
</tr>
<tr>
<td>Zero-order source term ($\gamma$)</td>
<td>0.0 m/L/day</td>
</tr>
<tr>
<td>Loading time ($t_0$)</td>
<td>1 day</td>
</tr>
<tr>
<td>Initial concentration ($C_i$)</td>
<td>0.0 mg/L</td>
</tr>
</tbody>
</table>

(b) saturated zone

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sand layer (upper)</strong></td>
<td><strong>Silty-Sand layer (lower)</strong></td>
</tr>
<tr>
<td>Hydraulic conductivity ($K$)</td>
<td>$1.5 \times 10^{-3}$ cm/s</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.25</td>
</tr>
<tr>
<td>Dispersivity ($a_L, a_T, a_V$)</td>
<td>9.0, 0.9, 0.09 m</td>
</tr>
<tr>
<td>Retardation factor ($R$)</td>
<td>1.0</td>
</tr>
<tr>
<td>First-order decay rates ($\mu$)</td>
<td>0.0 day$^{-1}$</td>
</tr>
</tbody>
</table>
**Table III-4.** Information for (a) the pumping wells and (b) the contaminant sources

(a) pumping wells

<table>
<thead>
<tr>
<th></th>
<th>Agricultural use</th>
<th>Domestic use</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RW</td>
<td>GW</td>
</tr>
<tr>
<td><strong>Pumping rates (m$^3$/day)</strong> $^1$</td>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td><strong>Water quality standard (mg/L)</strong> $^2$</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td><strong>Depth (m)</strong></td>
<td>10</td>
<td>30</td>
</tr>
</tbody>
</table>

(b) contaminant sources

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Area (m$^3$)</strong></td>
<td>14400</td>
<td>2700</td>
<td>14400</td>
<td>5400</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td><strong>Loading period (days)</strong></td>
<td>120</td>
<td>150</td>
<td>180</td>
<td>120</td>
<td>150</td>
<td>180</td>
</tr>
</tbody>
</table>

1) In Chapter III-3.2.3, pumping rates on all the wells were set to 0 m$^3$/day for simulating the no-pumping condition.

2) It followed the respective NO$_3$-N standards for agricultural and drinking water established by the Ministry of Environment in Korea.
3.2.2. Prediction under the condition of no-regulations

As a base case, drawdowns and concentrations for 10 years were predicted under the condition assuming no-regulations in pumping and contaminant loading. Pumping rates on the RWs \( (q_{RWs}) \) were assigned to 100 m\(^3\)/day, which was the pumping capacity of the large-scale agricultural pumps installed in the study area. On-ground contaminant loadings of 10 kg/10a, as much as the standard amount of nitrogen in fertilizer for lettuce that has mainly been grown in the greenhouses in the study area, were assigned for each loading period over the source areas. Because the standard amount of fertilizer was primarily established to apply an appropriate amount of fertilizer for enhancement of crop production, not for groundwater quality protection, the prediction under this condition might be to consider only the increase of agricultural income. As a result, the total revenue expected from the unregulated contaminant loading was estimated to be the maximum, \( 1.04 \times 10^6 \) [-] (Table III-5). However, in this prediction, concentrations in GW2 and GW3 were above the agricultural water quality standard and the maximum drawdowns on the three RWs, except for RW1, were more than 7 m.
Table III-5. Prediction result under the condition of no-regulations

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loading mass (kg)</td>
<td>144.0</td>
<td>27.0</td>
<td>144.0</td>
<td>54.0</td>
<td>18.0</td>
<td>27.0</td>
<td>414.0</td>
</tr>
<tr>
<td>M/A (kg/10a) 1)</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>-</td>
</tr>
<tr>
<td>Revenue (×10³, -)</td>
<td>432.0</td>
<td>64.8</td>
<td>288.0</td>
<td>162.0</td>
<td>43.2</td>
<td>54.0</td>
<td>1044.0</td>
</tr>
<tr>
<td>Wells violating C* 2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>GW3 (23.8 mg/L), GW2 (22.0 mg/L), GW1 (17.1 mg/L)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wells violating d* 3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>RW3 (9.25 m), RW2 (9.17 m), RW4 (7.87 m)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1) Loading mass/Area

2) Concentration constraint

3) Drawdown constraint
3.2.3. Optimal contaminant loading design under the no-pumping condition

The optimal design obtained under the no-pumping condition allowed the maximum amount of contaminant loadings, 10 kg/10a, on all the contaminant sources (Table III-6) although the depth of water table was kept shallowly under the condition of no-pumping and thus the aquifer must be vulnerable to the contaminant leaching from on-ground loading (Almasri and Kaluarachchi, 2004a). Furthermore, despite of the maximum of contaminant loading, the predicted maximum concentrations in most wells were far less than the water quality standards.

Figure III-10 illustrated a reason for these results of optimization and prediction. The contaminant plume moved along only the regional groundwater flow under the no-pumping condition but its pathway was just out of the distributions of the wells. In other words, because of such a plume pathway the wells were not exposed to the contamination seriously despite of the large amount of contaminant loading. However, the comparison with the results shown in the base case, which had assumed the same amount of contaminant loading with this optimal design after all but had considered the pumping condition, implies that an optimal contaminant loading design under the no-pumping condition could be inappropriate to apply in the
regions where has extracted groundwater of amount as much as assumed in the base case.

**Table III-6.** Optimization result obtained under the no-pumping condition

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Loading mass (kg)</strong></td>
<td>144.0</td>
<td>27.0</td>
<td>144.0</td>
<td>54.0</td>
<td>18.0</td>
<td>27.0</td>
<td>414.0</td>
</tr>
<tr>
<td><strong>M/A (kg/10a)</strong></td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>-</td>
</tr>
<tr>
<td><strong>Revenue (×10³, -)</strong></td>
<td>432.0</td>
<td>64.8</td>
<td>288.0</td>
<td>162.0</td>
<td>43.2</td>
<td>54.0</td>
<td>1044.0</td>
</tr>
<tr>
<td><strong>C max² in the wells</strong></td>
<td>GW3 (13.2 mg/L), GW2 (12.5 mg/L), RW2 (12.1 mg/L)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1) Loading mass/Area

2) Maximum concentration
Figure III-10. Simulation results applying the optimal contaminant loading mass determined under the no-pumping condition
3.2.4. Optimal contaminant loading design under the condition of pumping rates on the RWs = 100 m$^3$/day

Under the pumping conditions assumed in the base case (pumping rates on the RWs = 100 m$^3$/day), the optimal contaminant loading design was determined. The optimal permissible loading mass on the most influential source S1, which had the relative importance of 0.384 [-], was assigned to 7.8 kg/10a and the resulting maximum concentration in the GW3 was predicted to 19.9 mg/L. For the source S3 the contaminant loading mass close to the maximum, 9.9 kg/10a, was allowed although this source was second influential with the relative importance of 0.359. Nevertheless, its neighboring wells were not exposed to a serious contamination of concentrations above the water quality standards due to the relatively long loading period of 180 days as well as the water table depth declined by pumping, the locations of RWs, and the regional groundwater flow. The backward transport simulation result also presented that the sources S2, S5, and S6 had the relative importance of 0.043, 0.023, and 0.036, respectively. This result means that even if a large amount of contaminant loading were allowed on their sources it would rarely contaminate the wells and thus the determination of contaminant loading on these sources were actually
insignificant. All of these results were completely different from the previous results obtained under the no-pumping condition although the both designs were obtained under the same conditions, except for considering the groundwater pumping. This might imply an importance, or necessity, of considering pumping condition in determining the permissible on-ground contaminant loading, particularly in the agricultural regions where groundwater use has been common.
Table III-7. Optimization result obtained under the condition of pumping rates on the RWs = 100 m$^3$/day

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Loading mass (kg)</strong></td>
<td>112.6</td>
<td>21.6</td>
<td>142.7</td>
<td>53.5</td>
<td>18.0</td>
<td>27.0</td>
<td>375.4</td>
</tr>
<tr>
<td><strong>M/A (kg/10a)</strong> 1)</td>
<td>7.8</td>
<td>8.0</td>
<td>9.9</td>
<td>9.9</td>
<td>10.0</td>
<td>10.0</td>
<td>-</td>
</tr>
<tr>
<td><strong>Revenue (×10$^3$, -)</strong></td>
<td>337.7</td>
<td>51.8</td>
<td>285.4</td>
<td>160.5</td>
<td>43.2</td>
<td>54.0</td>
<td>932.7</td>
</tr>
<tr>
<td><strong>Relative Importance (-)</strong></td>
<td>0.384</td>
<td>0.043</td>
<td>0.359</td>
<td>0.155</td>
<td>0.023</td>
<td>0.036</td>
<td>-</td>
</tr>
<tr>
<td><strong>$C_{max}$ 2) in the wells</strong></td>
<td>GW3 (19.9 mg/L), GW2 (18.3 mg/L), DW2 (9.0 mg/L)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1) Loading mass/Area

2) Maximum concentration
4. Summary and conclusions

The management model for agricultural contaminant loading was
developed to determine the optimal permissible contaminant loading mass
possible to satisfy the both of economic and environmental demands for
groundwater use, using the simulation-optimization method. The field
investigation and observations introduced in the Chapter II were used in
developing the management model and evaluating its applicability. The 1-D
analytical model for solute transport in unsaturated zone was integrated with
the 3-D numerical model for groundwater flow and solute transport in
saturated zone in order to simulate groundwater contamination from
fertilizer application in greenhouse. The optimization technique, genetic
algorithm, was linked with the integrated simulation model to obtain to find
the optimal permissible on-ground contaminant loading mass. In addition,
the backward transport simulation procedure was added to the management
model in order to evaluate the relative importance of contaminant sources.
The case study for applicability of the backward transport simulation
procedure showed that its application was very useful in sorting out the
influential contaminant sources and managing those sources more
importantly. A part of the study area was chosen as the model domain and
the optimal permissible on-ground contaminant loading mass was determined on the greenhouses located at the site under several conditions of the groundwater flow. The results demonstrated that the developed model can be particularly helpful in obtaining the optimal contaminant loading design in agricultural regions where many possible non-point contaminant sources were distributed widely. In addition, it was shown that groundwater pumping should be considered in managing contaminant loading in agricultural region where a significant amount of groundwater has been used for agriculture.
CHAPTER IV. MODEL DEVELOPMENT FOR AGRICULTURAL CONTAMINANT LOADING MANAGEMENT WITH CONSIDERING PUMPING CONDITION

1. Introduction

In agricultural regions, a significant amount of groundwater has been used for agriculture due to its proximity while over-pumping has sometimes leaded to excessive drawdown and shortage of groundwater. However, agricultural activities, such as fertilizer application in the greenhouses, have often threatened groundwater quality or even sustainability for groundwater use (Postma et al., 1991; Baker, 1992; Chowdary et al., 2005; Almasri, 2007). Particularly, nitrate contamination of groundwater has a high correlation with nitrogen-based fertilizer applications (Joosten et al., 1998; Ling and El-Kadi, 1998; Harter et al., 2002; Shrestha and Ladha, 2002; Dunn et al., 2005; Jordan and Smith, 2005; Liu et al., 2005; Almasri, 2007). Many studies have developed several simulation and/or optimization models
to determine the optimal fertilizer application (van Genuchten, 1985; Wagenet and Hutson, 1987; Shaffer et al., 1991; HydroGeoLogic, 1996; Šimůnek et al., 1998, 1999a; Šimůnek et al., 1999b; Almasri and Kaluarachchi, 2005a; Jacques and Šimůnek, 2005; Peña-Haro et al., 2009, 2010; Trolldborg et al., 2009; Wei et al., 2009). However, only the fertilizer application does not affect the agricultural groundwater quality.

Groundwater pumping changes groundwater level and flow and, as a result, affects fate of solute in subsurface, such as leaching to the water table and migration in the aquifer. In the study area, paddy fields for rice farming, which generally require the large amount of water on its growing season, are wide spread on an alluvium. Although the Bokha stream is not far from the paddy field, most of farmers in this area have used groundwater for the rice farming because the small-scale of stream was not enough to satisfy all the demands for rice farming. In particular, $2.772 \times 10^6$ m$^3$/year of groundwater and more than 100 pumping wells was used for agriculture in this region (KOR MAF and KRC, 2006) and it might supported that the groundwater pumping for rice farming was one of the most significant factors affecting the groundwater quality in this study area. The results shown in the Chapter III already demonstrated that the optimal design for contaminant loading had been different according to the given pumping conditions. All of these
facts indicated that it is necessary to examine the effects and importance of pumping condition in determining the agricultural contaminant loading management and to find a methodology more appropriate to the agricultural regions where groundwater use has been common.

In this study, two approaches to consider pumping conditions in determining the optimal contaminant loading management were suggested: (1) a comparison of each optimal contaminant loading design obtained under the conditions of various pumping rates; and (2) a simultaneous optimization of contaminant loading and groundwater pumping. While for the former the model developed in the Chapter III could be used without any modification, for the latter a new model possible to optimize the loading mass together with pumping rates was developed.

2. Methodology

2.1. Comparison of optimal contaminant loading designs obtained under various pumping conditions

The optimal contaminant loading designs obtained under various pumping conditions were compared in order to examine effects of pumping
condition on determining the optimal contaminant loading and to find the best optimal design considering groundwater pumping among those designs. For this, the management model developed in the Chapter III was used. Although the model was developed to determine the optimal permissible contaminant loading mass, it could actually consider pumping conditions by assigning prespecified pumping rates on the wells in the groundwater flow and solute transport simulation model. Particularly, the calculated water table depths at the location of contaminant sources were used in the estimation of leaching mass. The details about the formulation of this simulation-optimization model were presented in the Chapter III-2.

2.2. Model development for simultaneous optimization of on-ground contaminant loading and pumping rates

A new simulation-optimization model possible to simultaneously optimize permissible on-ground contaminant loading mass and pumping rates was developed in this study. The basic structure of this model followed the model developed in the Chapter III. Particularly, the integrated simulation for unsaturated-saturated solute transport, the backward transport simulation for evaluating relative importance of contaminant sources, the
estimation of expected revenue, and the optimization using genetic algorithm were also applied to this model. However, in this optimization procedure, pumping rate on the RWs, or strictly pumping volume, was considered as another decision variable. Iteratively, it is generated with the loading mass and the both were evaluated together based on the objective function modified to consider the both, while only the loading mass was generated and evaluated in the previously developed model. The generated pumping rates on the RWs were first used in calculating the mean depth of water table at locations of the sources in order to estimate contaminant leaching mass together with the generated loading mass. Then, they were used in simulating the groundwater flow and contaminant migration in aquifer again. The modified objective function was formulated to maximize both of the permissible on-ground contaminant loading mass and the pumping volume, subject to constraints for drawdown and concentration. Particularly, the optimal pumping rate should be able to prevent well contamination as well as to supply a sufficient amount of groundwater and to prevent excessive drawdown. The objective function, the penalty function, and the constraints is given by
Maximize $fit_{\text{total}} = \left( \frac{c_1 \cdot \sum \omega_{\text{GH}} \cdot M_{\text{GH}} + c_2 \cdot \sum Q_{\text{RW}}}{c_p \cdot P} \right)$ \hspace{1mm} (IV-1)\\

subject to

$P = \left[ \max \left( 0, \frac{C_{\text{AW}}^{\text{max}} - C_{\text{AW}}^*}{\alpha_{\text{AW}}} \right) \right]^n + \left[ \max \left( 0, \frac{C_{\text{DW}}^{\text{max}} - C_{\text{DW}}^*}{\alpha_{\text{DW}}} \right) \right]^n + \left[ \max \left( 0, \frac{d^{\text{max}} - d^*}{\alpha_d} \right) \right]^n + \beta$ \hspace{1mm} (IV-2)

with constraints $C_{\text{AW}}^{\text{max}} < C_{\text{AW}}^*; \ C_{\text{DW}}^{\text{max}} < C_{\text{DW}}^*; \ d^{\text{max}} < d^*; q \leq q^*; \text{ and } M_{\text{GH}} \leq M^*$ \hspace{1mm} (IV-3)

where $fit_{\text{total}}$ is the total fitness value [-]; $P$ is the penalty value [-]; $\omega_{\text{GH}}$ is the weight of relative importance for each greenhouse group [-]; $M_{\text{GH}}$ is the permissible on-ground contaminant loading mass for each greenhouse group [M]; $Q_{\text{RW}}$ is the pumping volume on wells for rice agriculture [L$^3$], obtained by multiplying the pumping rates ($q$) [L$^3$T$^{-1}$] by the pumping time [T]; $c_1$, $c_2$, and $c_p$ are the cost coefficients for the contaminant loading [M$^{-1}$], the pumping [L$^{-3}$], and the penalty [-], respectively; $C_{\text{AW}}^{\text{max}}$ and $C_{\text{DW}}^{\text{max}}$ are the maximum concentrations in wells for agricultural use, located by rice paddies and greenhouses, and domestic wells, respectively [ML$^{-3}$]; $C_{\text{AW}}^*$
and $C_{DW}^*$ are the concentration constraints for agricultural and domestic use, respectively [ML$^{-3}$]; $d_{\text{max}}$ is the calculated maximum drawdown in the wells [L]; $d^*$ is the drawdown constraint [L]; $\alpha_{AWC}$, $\alpha_{DWC}$, and $\alpha_d$, are the violation allowances for the concentrations in agricultural and domestic wells and drawdown, respectively [-]; $n$ is the coefficient for magnifying each penalty value exponentially [-]; $\beta$ is a constant to ensure that the denominator of the objective function is non-zero [-]; $q^*$ is the pumping rate constraint [L$^3$T$^{-1}$]; and $M^*$ is the loading mass constraint [M]. The overall simulation-optimization procedure was shown in Figure IV-1.
Figure IV-1. Flow chart of the management process in the model developed to optimize on-ground contaminant loading together with pumping rates.
3. Results and Discussion

The model domain based on the study area, introduced in the Chapter III-3.2 and Figure III-9, was used to demonstrate the optimization results of the both management approaches suggested in this study again.

3.1. Optimal contaminant loading designs obtained under various pumping condition

To quantitatively examine the effects of pumping conditions in determining the optimal contaminant loading management, the optimal designs for contaminant loading obtained under various pumping conditions were compared. The range of pumping rates on the RWs \((q_{\text{RWs}})\) considered for the comparison was from 10 to 100 m\(^3\)/day and the optimal contaminant loading designs were respectively determined with each rates of pumping on the RWs.

Figure IV-2 illustrates that the optimal designs were determined differently with the given pumping rates of the RWs. A general tendency that more loading mass were allowed with increasing pumping rates of the RWs was found in S1 and S3, which were the most influential sources on
the wells in all the optimal designs (Figure IV-3). About this tendency, Figure IV-4 shows that increasing pumping rates caused the water table to lower and, as a result, the maximum contaminant leaching mass decreased gradually. In other words, due to the decline of water table with increasing pumping rates, both distance and duration for leaching from the ground to the water table increases and, as a result, more dispersed contaminants leaches to the water table. Therefore, the optimal designs obtained under the large rates of pumping conditions suggested that restrictions of contaminant loading were hardly necessary. On the other hand, under the low rates of pumping conditions ($q_{RWs} = 10–20 \text{ m}^3/\text{day}$), the optimal designs was suggested to restrict the contaminant loading considerably because shallow aquifers kept under low rates of pumping conditions must be more vulnerable to contaminant leaching (Almasri and Kaluarachchi, 2004a). Moreover, the pumping on those wells also affected the groundwater flow and the resulting contaminant migration in the aquifer. The change in optimal loading mass suggested for S1 included a sudden increase at $q_{RWs} = 40 \text{ m}^3/\text{day}$ and a slight decrease in the range of $q_{RWs} = 40–70 \text{ m}^3/\text{day}$ despite of the increase of pumping rates (Figure IV-2), and was distinct from that of S3 increasing monotonically with pumping rates. Particularly, at $q_{RWs} = 40 \text{ m}^3/\text{day}$, the maximum concentration in DW1, which had mainly limited the
contaminant loading of S1 in most of the designs because of the stricter constraint assigned on this well, were exceptionally low (5.1 mg/L), while the maximum concentrations in GW2, GW3, and RW2 were rather higher than those under other pumping conditions (17.8, 19.8, and 13.4 mg/L, respectively). The similar phenomenon was also found in the optimal design at $q_{RWs} = 100$ m$^3$/day, which caused the largest drawdown and the strongest inflow to the RWs. These results implies that the groundwater flow field created by these rates of pumping in the RWs, particularly RW2, might lead to a horizontal migration of contaminant plume into GW2, GW3, and RWs located at the downgradient. In addition, the pumping conditions in the range of $q_{RWs} = 40–70$ m$^3$/day might create groundwater flow fields such that the contaminant plume from S1 would enter DW1 more strongly with increasing pumping rates.

The revenues expected to be obtained from the fertilizer applications corresponding to these optimal designs were calculated (Figure IV-5). Similarly to the tendency mentioned previously, the total of expected revenues also increased gradually with the pumping rates and, thus, the optimal design at $q_{RWs} = 100$ m$^3$/day was expected to obtain the most revenue, $9.33 \times 10^5$ [-]. However, this design might be inappropriate in preserving groundwater quantity although having protected groundwater
quality successfully and maximized the expected revenue; it had resulted in excessive drawdown, i.e., 9.25 m in RW3. Consequently, the optimal loading design at $q_{RWs} = 70 \text{ m}^3/\text{day}$ having the expected revenue of $7.86 \times 10^5 [-]$, which also satisfied the drawdown constraint, could be most appropriate and efficient.
Figure IV-2. Changes in the optimal contaminant loading mass on the sources according to the given pumping rates on the RWs.
Figure IV-3. Relative importance of contaminant sources according to the given pumping rates on the RWs
Figure IV-4. 10-day averaged maximum leaching mass and area-averaged depth to the water table located below S1 calculated from each contaminant loading design according to the given pumping rates on the RWs.
Figure IV-5. Changes in the total expected revenues according to the given pumping rates on the RWs.
The effects of pumping condition in determining optimal contaminant loading were also examined under the condition that the constant head boundary at right side was modified to 44.0 m. As a result, the water table became deeper over the domain than the previous one and the hydraulic gradient was about 0.008 under the condition without any pumping. While the tendency similar to the previous one shown in Figure IV-2 was also found in Figure IV-6, the sudden increase in the optimal contaminant loading mass suggested for \( q_{RWs} = 40 \text{ m}^3/\text{day} \) were greater than the previous one obtained at the same pumping rates. This result might imply that the water table deepened due to the modification of boundary condition leaded to the more dispersed leaching and the larger hydraulic gradient resulted in a stronger horizontal migration into the pumping wells located at the downgradient of S1 than the previous one. This modification of boundary condition also affected on the total expected revenues. Among the optimal designs that satisfying the drawdown constraint, the optimal designs at \( q_{RWs} = 40 \text{ m}^3/\text{day} \) was expected to obtain the most revenues, \( 7.78 \times 10^5 \) [-], as shown in Figure IV-7. This result demonstrated that more rates of pumping might not always allow an increase in the expected revenues and it is very important to consider pumping conditions because groundwater pumping under a specific flow condition can have a more significant influence in
determining the optimal contaminant loading.

**Figure IV-6.** Changes of the optimal contaminant loading mass on the sources according to the given pumping rates on the RWs under the condition that the constant head boundary at the right side was set to 44.0 m
Figure IV-7. Changes in the total expected revenues according to the given pumping rates on the RWs under the condition that the constant head boundary at the right side was set to 44.0 m
3.2 Simultaneous optimization of on-ground contaminant loading and pumping rates

The approach of comparing the optimal designs determined under different pumping conditions may actually be the simplest way to find the best contaminant loading design with consideration of pumping conditions. The model developed in the Chapter III is capable of managing agricultural contaminant loading under a specified pumping condition. However, as well as requiring too much computational time and efforts, this approach cannot consider neither complicated dynamics between fate of contaminants and pumping nor various conditions such as different usage of, or demand on, each pumping well and contaminant source. To overcome these problems, pumping rates on the RWs were simultaneously optimized together with permissible on-ground contaminant loading mass using the management model introduced in this chapter. The range of $q_{RWs}$, as another decision variable, for the optimization was from 30 to 120 m$^3$/day. In the optimization, the drawdown constraint was set to 7 m, which was the installation depth of most of the agricultural wells located in the study area. Information about the pumping wells and contaminant sources were shown in Tables IV-1.
The optimal design for pumping assigned the rates of 50, 50, and 90 m$^3$/day on RW2, RW3, and RW4, respectively. But the pumping rate of RW1, which was located upgradient of the contaminant source S1, was suggested to increase by 110 m$^3$/day and, as a result, the highest drawdown was 6.74 m on this well (Table IV-2). The total amount of groundwater supply expected in this design was greater than that expected from the optimal design at $q_{RW_s} = 70$ m$^3$/day, which had been the best design in the Chapter IV-3.1. Even though this optimal design allowed more loading mass on the S1, 5.7 kg/10a, concentrations in all wells were predicted to be kept below the water quality standards, and this implies that the suggested pumping design also had an important role to prevent well contamination.
Table IV-1. Information for (a) the pumping wells and (b) the contaminant source

(a) pumping wells

<table>
<thead>
<tr>
<th></th>
<th>Agricultural use</th>
<th>Domestic use</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RW</td>
<td>GW</td>
</tr>
<tr>
<td>Pumping rates (m³/day)</td>
<td>30–120 ²)</td>
<td>10</td>
</tr>
<tr>
<td>Water quality standard (mg/L) ¹)</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td>Depth (m)</td>
<td>10</td>
<td>30</td>
</tr>
</tbody>
</table>

(b) contaminant source

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area (m³)</td>
<td>14400</td>
<td>2700</td>
<td>14400</td>
<td>5400</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td>Loading period (days)</td>
<td>120</td>
<td>150</td>
<td>180</td>
<td>120</td>
<td>150</td>
<td>180</td>
</tr>
</tbody>
</table>

¹) It followed the respective NO₃-N standards for agricultural and drinking water established by the Ministry of Environment in Korea.

²) The pumping rates on the RWs were used as decision variables.
Table IV-2. Optimization result for determining permissible contaminant loading mass together with pumping rates on the RWs

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Loading mass (kg)</strong></td>
<td>82.5</td>
<td>22.6</td>
<td>144.0</td>
<td>43.2</td>
<td>18.0</td>
<td>12.3</td>
<td>322.6</td>
</tr>
<tr>
<td><strong>M/A (kg/10a)</strong></td>
<td>5.7</td>
<td>8.4</td>
<td>10.0</td>
<td>8.0</td>
<td>10.0</td>
<td>4.5</td>
<td>-</td>
</tr>
<tr>
<td><strong>Revenue (×10³, -)</strong></td>
<td>247.4</td>
<td>54.2</td>
<td>288.0</td>
<td>129.6</td>
<td>43.2</td>
<td>24.5</td>
<td>787.0</td>
</tr>
<tr>
<td><strong>Relative importance (-)</strong></td>
<td>0.379</td>
<td>0.041</td>
<td>0.381</td>
<td>0.137</td>
<td>0.021</td>
<td>0.040</td>
<td>-</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>RW1</th>
<th>RW2</th>
<th>RW3</th>
<th>RW4</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pumping rates (m³/day)</strong></td>
<td>110.0</td>
<td>50.0</td>
<td>50.0</td>
<td>90.0</td>
</tr>
</tbody>
</table>
4. **Summary and conclusions**

In this chapter, the effects of pumping conditions in determining the contaminant loading management were examined quantitatively, based on the followings: (1) groundwater has been commonly used in most of the agricultural regions where have often a problem in groundwater quality due to agricultural activities, (2) groundwater pumping can significantly affect fate of on-ground loaded contaminant, and (3) the optimal contaminant loading designs obtained in the Chapter III had been different with consideration of pumping condition. For this, the optimal contaminant loading designs were obtained under various pumping conditions using the management model developed in the Chapter III. The comparison of those optimal designs demonstrated that agricultural contaminant loading management can be determined differently according to the given pumping conditions. Particularly, while more contaminant loading was mostly allowed with increasing pumping rates, the optimal contaminant loading mass determined on some source fluctuated with increasing pumping rates. In addition, the result obtained by modifying the boundary condition showed that the consideration of pumping condition could be more significant in contaminant loading management in a specific
hydrogeological condition. All of these results indicated that for the more appropriate agricultural contaminant loading management, it is definitely necessary to consider pumping condition.

Furthermore, the management model to simultaneously optimize both of the permissible contaminant loading mass and pumping rates was developed. The objective function was formulated to allow a sufficient amount of on-ground contaminant loading and groundwater supply as well as to prevent well contamination and excessive drawdown. This model cannot consider only complicated dynamics between fate of contaminant and pumping but also various conditions such as different usage of, or demand on, each pumping well and contaminant source in a single of optimization process. The optimal design determined from this model allowed more amounts of both of contaminant loading and groundwater pumping than any other optimal design suggested previously. The developed model can be useful in the contaminant loading management in the agricultural regions where groundwater has been extensively used for agriculture.
CHAPTER V. MODEL DEVELOPMENT FOR AGRICULTURAL CONTAMINANT LOADING MANAGEMENT UNDER THE TIME-VARIANT PUMPING CONDITION

1. Introduction

In the agricultural regions where groundwater use has been concentrated in a specific period of time, it is particularly important to consider the pumping conditions in managing contaminant loading. For example, in the study area where rice paddy fields are widespread, a significant amount of water for rice farming is required during its growing season and most or a large portion of the required water has come from groundwater because of its spatial proximity and availability. As a result, groundwater level and flow must have been changed from season to season and so does the fate of agricultural contaminant in the subsurface zone. This indicates that the fate of contaminants according to the seasonal pumping should be considered in determining contaminant loading management in
those regions. For this, however, the contaminant leaching to the water table fluctuated by the time-variant pumping is necessary to be simulated as well as the transient groundwater flow and the resulting contaminant transport.

Many analytical and numerical models have been developed to simulate solute transport in the unsaturated zone. However, they computed the leaching mass to only the water table at a fixed depth and only a few models could simulate the leaching under transient flow condition caused by precipitation (van Genuchten, 1985; Wagenet and Hutson, 1987; Shaffer et al., 1991; HydroGeoLogic, 1996; Šimůnek et al., 1998, 1999a,b; Jacques and Šimůnek, 2005; Troldborg et al., 2009). Actually, it is very difficult and complicated to explicitly simulate the solute leaching to the water table fluctuated by pumping using only the existing unsaturated transport model (Legout et al. 2009); it can neither predict changes in the groundwater level by pumping nor calculate the leaching mass changed according to those predictions. Thus, it was necessary to suggest another approach possible to predict or approximate the leaching to the fluctuating water table.

The objective of this study was to develop the management model to determine the optimal agricultural contaminant loading more appropriate to the regions where groundwater has been used intensively in a specific period. For this, a method to approximate contaminant leaching to the water
Table fluctuated by groundwater pumping with the transient groundwater flow simulation were suggested to simulate the fate of contaminants under the time-variant pumping conditions.

2. Methodology

2.1. Approximation of the leaching to fluctuating water table under time-variant pumping condition

Two techniques were proposed in order to approximate the solute leaching to the water table that fluctuates regularly with a seasonal pumping schedule: (1) application of the analytical solution, which is simple and easy to handle for both simulation and optimization; and (2) combination of the respective breakthrough curves describing the leaching at each different depth and status of water table (Figure V-1). For the former, the analytical solution suggested by van Genuchten (1981) was applied. It was assumed that contaminant does not have any reaction in the unsaturated zone and will be dissolved immediately if it reaches the water table. The details of this solution were introduced in van Genuchten (1981) and in the Chapter III. For the latter, the ways to combine breakthrough curves are differently
suggested according to the changing pattern of water table depth due to a given pumping schedule within a single of loading period. For the case that pumping starts within a single of loading period, first, it derives breakthrough curves for a given on-ground contaminant loading mass at the stable depths of water table created before and during the pumping respectively, using the analytical solution. The desired breakthrough curve for the time before the pumping just follows the curve derived at the stable depth kept before pumping and the corresponding total leaching mass for this time is $M_1$, which can be calculated by integrating the breakthrough curve over this time. There would be no leaching to the on-falling water table for a certain time after the pumping starts, as solutes generally move downward more slowly than the falling water table. The period of no leaching was determined from the fact that only the remaining mass ($M_2$), excluding the leaching mass to the water table before the pumping ($M_1$) from the total mass of this loading ($M_{total}$), would leach to the declined water table after pumping ($M_2 = M_{total} - M_1$). The desired breakthrough curve for the time after the water table declined by pumping becomes stable also follows the one derived at the stable depth kept during the pumping but it starts from the time that integration of this curve from the initial time became equal to the $M_1$ (Figure V-1(a)). For the case that pumping stops
within a single of loading period, similarly to the above procedure, the
desired breakthrough curves follows the curves respectively derived at the
stable depths of water table kept during the pumping and after its stopping.
However, the leaching mass to the recovering water table right after
stopping the pumping can be obtained by adding the two following
components for each time step: ① for \( i \)-th time step \( t_i \), the mass of the solute
already located at the depth of water table \( d_i \) to the depth predicted at next
time step \( d_{i+1} \); ② during the period from \( t_i \) to \( t_{i+1} \), the mass of the solute
leaching to the next depth \( d_{i+1} \) of water table. The former is the mass
predicted by only the recovery of the water table, the latter is the mass
predicted by only the downward movement of the solute. These procedures
suggested for the two cases were just the basic structures for the
approximation of leaching mass to the water table fluctuated by the time-
variant pumping. Actually, it was necessary to identify various patterns and
timing of water table fluctuation by such pumping schedule within each
single of loading period and to combine the breakthrough curves in
accordance with each situation because there are usually a discrepancy
between the loading period and the seasonal pumping schedule. Actually, 12
typical patterns of water table fluctuation caused by a given pumping
schedule within a single of loading event were considered (Figure V-2) and
the ways to derive the breakthrough curves according to those patterns was devised respectively based on the suggested procedures. **Figure V-3** presented some examples of breakthrough curves obtained according to the typical patterns of water table fluctuation.
**Figure V-1.** Schematic diagram of obtaining the mass leaching to the fluctuating water table through combining the breakthrough curves
Figure V-2. Typical patterns of water table fluctuation according to the seasonal pumping schedule within a single contaminant loading period
Figure V-3. Examples of leaching mass approximated according to the typical patterns of water table fluctuation
2.2. Simulation-optimization model for the agricultural contaminant loading management under time-variant pumping condition

The transient groundwater flow simulation was applied to predict and identify the water table fluctuation caused by seasonal pumping and the resulting contaminant leaching and migration in the aquifer. The details about the governing equations for groundwater flow and forward (general)/backward solute transport were already demonstrated in the Chapter III and they were simulated using Hydrogeosphere, which is the numerical model that can simulate all these procedures (Therrien et al., 2010). For the simultaneous optimization of permissible contaminant loading mass and pumping rates, the genetic algorithm was linked to the integrated simulation model. The objective function for pumping was modified a little, which was to maximize the pumping volume during only the specified period. The entire simulation-optimization procedure developed in this study was demonstrated in Figure V-4.
Start
Generation of initial decision variables (q, M)
Fitness evaluation
Does it satisfy stopping criteria?
Optimal design
End

Calculation of states variables (h, C)

Pumping rates (q)
Depth of water table
Leaching mass

2. Hydrogeosphere, Therrien et al., 2010

Figure V-4. Flow chart of the management process in the model developed for the agricultural contaminant loading management under the time-variant pumping condition
3. Results and discussion

3.1. Estimation results of the leaching mass to fluctuating water table

Seasonal pumping operations would completely change fate of contaminant as well as depth of water table. In the case of no-regulation presented in the Chapter III-3.2.2, assuming that $q_{RWS} = 100 \text{ m}^3/\text{day}$ and contaminant loading mass on all the sources = 10 kg/10a, leaching mass flux from periodical contaminant loading on S1 was estimated under the time-invariant condition. In this simulation, the pumps on the RWs were assumed to be operated from May to August. The water table located below the contaminant sources was predicted to fluctuate in a range of about 2–4 m in the simulation time (Figure V-5). The patterns of fluctuating water table shown during the time of each single contaminant loading was found to be various and complicated due to the discrepancy between the seasonal pumping schedule and the contaminant loading period of each source. For example, while after 18-th contaminant loading (2040 days) the water table that had been declined by the pumping on the RWs was recovered by stopping the pumping and then became stable, the water table that had been kept shallow without the pumping on the RWs declined by starting the
pumping after 19-th contaminant loading (2160 days) and then became stable (Figure V-6). Figure V-7 shows the breakthrough curves of leaching mass obtained from each periodical contaminant loading on S1 in the time of 2000-3000 days. Particularly, the sharply peaks of leaching were predicted from 18, 21, and 24-th contaminant loading and it is because the water table was recovered immediately due to stopping the pumping on the RWs soon after those contaminant loading.
Figure V-5. Changes in areal-averaged hydraulic heads in the locations of contaminant sources.
Figure V-6. Areal-averaged hydraulic heads at the S1 from 2000 to 3000 days and the patterns of water table fluctuation shown within each period of contaminant loading, shown in Figure V-2.
Figure V-7. Breakthrough curves for contaminant leaching obtained from the periodical loading on S1 and seasonal pumping operation in the time of 2000-3000 days.
3.2. Simulation and optimization results obtained under time-variant pumping condition

In the Chapters III and IV, all the optimal designs were obtained under time-invariant pumping conditions with steady-state flow simulations. However, they might sometimes be inappropriate in some agricultural regions, requiring a significant amount of groundwater seasonally, because they cannot consider any effect of time-variant pumping on the fate of the contaminant loaded on ground surface. Some of the previous designs were re-simulated under the condition of seasonal pumping for the transient-state flow system. For this, the pumps in RWs were assumed to be operated only from May to August, imitating the rice-growing season, for 10 years. For the no-regulation case presented in the Chapter III-3.2.2, more severe contamination was predicted in the wells than that of the previous prediction; a total of eleven wells including two DWs violated their respective water quality standards. The highest concentration was calculated to 39.5 mg/L in GW3 (Table V-1(a)), while it had been 25.4 mg/L under the time-invariant pumping condition (Table III-5). Even the optimal design that had determined pumping rates and permissible on-ground contaminant loading mass simultaneously (Table IV-2), suggested in the Chapter IV-3.2,
was also predicted to fail under this seasonal pumping condition, with a total of eight wells, including two DWs, contaminated (Table V-1(b)). In both of the results, the calculated maximum drawdowns were same with those predicted under the time-invariant pumping condition but it was obvious that the groundwater level and flow was completely different according to the seasonal pumping condition over the simulation time.

In order to determine the contaminant loading appropriate to the time-variant pumping condition, permissible on-ground contaminant loading mass and pumping rates for the RWs were simultaneously optimized using the transient-flow simulation and the method suggested to approximate contaminant leaching to a fluctuating water table. The range of the $q_{RWs}$ for the specific period of time as a decision variable for the optimization was from 30 to 120 m$^3$/day. In the optimizations, the drawdown constraint was set to 7 m, which was the installation depth of most of the agricultural wells located in the study area. Information about the pumping wells and contaminant sources were summarized in Tables V-2. The optimal $q_{RWs}$ were suggested to be 110, 60, 60, and 90 m$^3$/day respectively during the periods when the groundwater was extracted on the RWs (Table V-3). The permissible on-ground contaminant loading mass should be reduced by at least more than 30% of the maximum on most of the contaminant sources.
As a result, the total revenue was just about 47% of that of the no-regulation case shown in the Chapter III-3.2.2 (Table III-5). The maximum concentration in DW1 was very close to the standard, despite a contaminant loading of only 3.6 kg/10a on S1.

The inappropriateness of the optimal designs determined with the steady-state flow simulations and the strong restriction of contaminant loading in the optimal design considering the time-variant pumping conditions could be explained with the following simulation results: (1) because of the relatively shallow depth of water table kept during the period when the pumps in RWs were not being operated, the on-ground loaded contaminants may leach to the water table in less dispersed and higher concentrations (Figure V-8) (2) the periodical peaks shown in Figure V-9 appeared at the periods with pumping on the RWs, possibly proving that the contaminant plume can be driven into the wells intensively by a larger amount of pumping during only its operation; and (3) the sharply high concentration of contaminant leaching showed that the on-ground loaded contaminants sometimes suddenly leached to the recovering water table, immediately after stopping pumping (Figure V-8).
Table V-1. Simulation results under the time-variant pumping condition of (a) the no-pumping case (Chapter III-3.2.2) and (b) the design to simultaneously optimize pumping rates and loading mass under the time-invariant condition (Chapter IV-3.2)

<table>
<thead>
<tr>
<th>Wells violating $C^*$</th>
<th>$C^{max}$ (mg/L)</th>
<th>Wells violating $C^*$</th>
<th>$C^{max}$ (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GW1</td>
<td>27.2</td>
<td>GW2</td>
<td>24.3</td>
</tr>
<tr>
<td>GW2</td>
<td>36.7</td>
<td>GW3</td>
<td>26.0</td>
</tr>
<tr>
<td>GW3</td>
<td>39.5</td>
<td>GW5</td>
<td>26.9</td>
</tr>
<tr>
<td>GW4</td>
<td>22.2</td>
<td>GW8</td>
<td>23.7</td>
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<td>22.7</td>
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<td>GW9</td>
<td>23.9</td>
<td>DW1</td>
<td>14.2</td>
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<tr>
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<td>25.1</td>
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<td>RW2</td>
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<td></td>
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</tr>
<tr>
<td>DW1</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>DW2</td>
<td>13.3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1) Pumping rates  
2) Loading mass
Table V-2. Information for (a) the pumping wells and (b) the contaminant source

(a) pumping wells

<table>
<thead>
<tr>
<th></th>
<th>Agricultural use</th>
<th>Domestic use</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RW</td>
<td>GW</td>
</tr>
<tr>
<td><strong>Pumping rates (m³/day)</strong></td>
<td>30–120</td>
<td>10</td>
</tr>
<tr>
<td><strong>Pumping period</strong></td>
<td>May–August</td>
<td>everyday</td>
</tr>
<tr>
<td><strong>Water quality standard (mg/L)</strong></td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td><strong>Depth (m)</strong></td>
<td>10</td>
<td>30</td>
</tr>
</tbody>
</table>

(b) contaminant source

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Area (m³)</strong></td>
<td>14400</td>
<td>2700</td>
<td>14400</td>
<td>5400</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td><strong>Loading period (days)</strong></td>
<td>120</td>
<td>150</td>
<td>180</td>
<td>120</td>
<td>150</td>
<td>180</td>
</tr>
</tbody>
</table>

1) It followed the respective NO₃-N standards for agricultural and drinking water established by the Ministry of Environment in Korea.

2) The pumping rates on the RWs were used as decision variables.

3) This pumping period was considered as rice-growing season.
Table V-3. Optimization result for permissible contaminant loading mass and pumping rates on the RWs under time-variant pumping conditions

<table>
<thead>
<tr>
<th></th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
<th>S6</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loading mass (kg)</td>
<td>52.4</td>
<td>20.4</td>
<td>99.5</td>
<td>21.6</td>
<td>18.0</td>
<td>27.0</td>
<td>238.9</td>
</tr>
<tr>
<td>M/A (kg/10a)</td>
<td>3.6</td>
<td>7.6</td>
<td>6.9</td>
<td>4.0</td>
<td>10.0</td>
<td>10.0</td>
<td>-</td>
</tr>
<tr>
<td>Revenue (×10³, -)</td>
<td>157.1</td>
<td>48.9</td>
<td>199.0</td>
<td>64.8</td>
<td>43.2</td>
<td>54.0</td>
<td>567.0</td>
</tr>
<tr>
<td>Relative importance (-)</td>
<td>0.379</td>
<td>0.042</td>
<td>0.378</td>
<td>0.143</td>
<td>0.022</td>
<td>0.038</td>
<td>-</td>
</tr>
<tr>
<td>Pumping rates (m³/day)</td>
<td>110.0</td>
<td>60.0</td>
<td>60.0</td>
<td>90.0</td>
<td></td>
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Figure V-8. 10-day averaged leaching mass predicted from the contaminant loading of 10 kg/10a on S1 under (a) no-pumping, (b) time-invariant pumping, and (c) time-variant pumping conditions. In (b) and (c), it was assumed that $q_{RWS} = 100 \text{ m}^3/\text{day}$
Figure V-9. Concentrations in GW9 predicted from the contaminant loading of 10 kg/10a on S3 under (a) no-pumping, (b) time-invariant pumping, and (c) time-variant pumping conditions. In (b) and (c), it was assumed that $q_{RWS} = 100 \text{ m}^3/\text{day}$
3.3. Contaminant loading management without considering pumping conditions

The optimal contaminant loading design obtained under the no-pumping condition might be identical to the optimal design determined without considering pumping condition. In other words, the optimal design under the no-pumping condition suggested in the Chapter III-3.2.3 was actually to follow the same process with the comprehensive studies on agricultural contaminant loading management that had not considered any effect of pumping condition on the fate of contaminant, for example Almasri and Kaluarachchi (2005) and Peña-Haro et al. (2009, 2010). Suppose that the optimal design obtained under the no-pumping condition will really be applied to the agricultural regions that groundwater has been commonly used. This design suggested allowing the maximum loading mass on all contaminant sources because the contaminant plumes from those sources were predicted to migrate out of the distribution of wells, although the aquifer must be most vulnerable to the on-ground contaminant loading because of its shallow depth under the no-pumping condition (Almasri and Kaluarachchi, 2004a). However, as shown in Chapter IV-3.1, the optimal designs obtained under the conditions of low pumping rates demonstrated
that contaminant loading should be restricted considerably due to the small amount of groundwater pumping. Particularly, the optimal design for the pumping conditions of $q_{RWs} = 10 \text{ m}^3/\text{day}$ suggested the strictest restriction in contaminant loading among the optimal designs obtained under the time-invariant pumping conditions (Figure IV-2). While the high concentration of contaminants might leach to the water table because the aquifer under these pumping conditions must be as shallow as one under the condition of no-pumping, the low rates of pumping must lead to inflow of such contaminants toward the wells significantly. In other words, when it applies the optimal design obtained without considering pumping condition to the agricultural regions using groundwater, a serious contamination unpredicted in the design can be detected on the wells. This also implies that the shallow aquifers can become more vulnerable to the agricultural contaminant loading due to the pumping condition.

**Figure V-8** demonstrated that the optimal design obtained without considering pumping condition might more severely threaten groundwater quality in the agricultural regions where groundwater use has been concentrated seasonally. For a given condition of $q_{RWs} = 100 \text{ m}^3/\text{day}$, the leaching mass estimated under the seasonal pumping schedule was always more than that estimated under the time-invariant pumping condition.
because the water table was kept shallow during the period when the pumps on RWs were not operated. Particularly, the maximum leaching mass estimated under this time-variant pumping condition was 0.597 kg/day/a at an around 3161 days, which resulted from the sudden leaching of downward-moving contaminants to the recovering water table after stopping the operation of pump on the RWs.

For the given on-ground contaminant loading of 10kg/10a on S3, the concentration in GW9 predicted under the no-pumping condition might be an underestimation as compared with one predicted with considering pumping conditions (Figure V-9). Under the no-pumping condition, the concentration in GW9 increased gradually with time, which was 6.3 mg/L at around 3650 days and increased to 15.9 mg/L at the end of simulation. However, under the time-invariant pumping condition of \( q_{RWS} = 100 \text{ m}^3/\text{day} \), despite of its relatively small amount of leaching, the concentration in GW9 was higher than that predicted under the no-pumping condition over the whole simulation time. Particularly, the concentration in GW9 already increased to 16.5 mg/L at around 1411 days and then became steady with a fluctuation, which indicated the effect of periodical contaminant loading on S3 on the GW9. The concentration predicted under the time-variant condition of seasonal pumping schedule increased by 26.0 mg/L at around
2800 days and then be also steady with another period of fluctuation, which was correspondent to the times when the pumps on the RWs were being operated. Particularly, the peak concentrations were appeared during those times. All of these results were concluded that a contaminant loading management without considering pumping condition must be inappropriate in the agricultural regions that groundwater has been used intensively and/or extensively.

In addition, regional groundwater flow field can also affect management policy in relation to other water bodies. Figure III-10 shows that under no-pumping condition, the plume with concentrations much greater than 10 mg/L would reach the right boundary of domain within 10 years while it was not observed in the wells. In other words, without suitable management, the contaminant plume might proceed into the adjacent water body with the regional groundwater flow. However, under the conditions with groundwater pumping, the plume would be unlikely to leave the domain owing to pumping from the wells (e.g., Figure V-10).
Figure V-10. Simulation results applying the optimal contaminant loading mass determined under the time-invariant pumping condition of $q_{RWS} = 100$ m$^3$/day
4. Summary and conclusions

In this chapter, the management model to determine the optimal design for contaminant loading and groundwater pumping under the time-variant conditions was developed with the method to approximate the leaching mass to the water table fluctuated by such pumping schedule and the transient flow simulation. In the method for the estimation of leaching mass under the time-variant pumping condition, the respective derived breakthrough curves were combined corresponding to each pattern and time of the water table fluctuation, and then reproduced to a single integrated breakthrough curve describing overall solute leaching. The optimal design using this developed model suggested that the contaminant loading should be restricted significantly under the time-variant pumping condition. The simulation results under the time-variant pumping condition presented three important reasons for the restriction of contaminant loading, which were the contaminant leaching to the shallow depth of water table kept during the period when the pumps in RWs were not being operated, a sudden increase of contaminant leaching to the water table recovering immediately after stopping the pumping on the RWs, and the inflow of contaminant plume to the wells driven by the large amount of pumping on the RWs for a specific
time of period. The importance of considering the pumping condition in the contaminant loading management was also demonstrated. While the previous studies for agricultural contaminant loading management did not consider any pumping condition, this study showed that the optimal design under the no-pumping condition could be failed in the regions that groundwater has been used commonly. Particularly, in the agricultural regions where a significant amount of groundwater has been extracted intensively for a specific time of period, like the study area, it was predicted that the optimal design obtained under the time-variant condition might lead to a serious and unpredicted contamination on the wells as well as the design obtained under the no-pumping condition. The model developed in this study is expected to be useful in the agricultural contaminant loading management in those agricultural regions.
DISCUSSION

The methodologies developed in this study followed the general conceptual simulation and management frameworks for predicting and controlling nitrate contamination in groundwater suggested by Almasri and Kaluarachchi (2007) and Almasri (2007). Land use and nitrogen source assessment was carried out in several times of field investigations in the study area and the fertilizer application in greenhouse which is periodical and on-ground loading of contaminant source were considered as a management target. The simulation model integrating the respective solute transport models in unsaturated and saturated zone can evaluate nitrate leaching to groundwater from periodical on-ground loading, migration of nitrate along with groundwater flow, and potential effects on the surface water body. The optimization model linked to the integrated simulation model can determine the optimal fertilizer application rates to maximize agricultural productivity and income while to preserve groundwater quality. However, throughout this study, it was demonstrated that groundwater pumping is critical in fate of nitrate in the subsurface zone. Therefore, its prediction and management without considering groundwater pumping can be unrealistic (Park et al., 2014), while almost all the previous studies about
agricultural contamination management have seldom considered effects of groundwater pumping. To the best of my knowledge the simulation-optimization models developed in this study are the only one possible to consider groundwater pumping in the agricultural contamination management. This study and the developed models must be useful to establish more practical groundwater contamination management plan in many agricultural regions where groundwater has been used extensively and commonly.

Nevertheless, some improvements are still required in this study in order to understand all of the participants related to the agricultural contamination management, including farmers and villagers, policy maker, stakeholder, and NGO, and to suggest a balanced solution to them having conflicting objectives and demands. Actually, they might have interested mainly in the final decision of management option rather than understanding of fate of nitrate in subsurface zone or simulation-optimization process in the developed model: for examples, which nitrogen source should be managed or when, where, and what amount of fertilizer application would be allowed. However, the simulation model for fate of nitrate in the subsurface zone must be still a powerful tool to quantitatively assess environmental effects according to each management option and to provide
scientific evidences in determining the best management option. Therefore, nitrate contamination prediction should be more accurate, realistic, and reliable than that shown in this study by configuring all the nitrogen sources and pumping wells spatially distributed in the region, reflecting actual information for different type of agricultural contaminant loading on the model, considering nitrogen dynamics in the unsaturated/saturated zone, simulating groundwater flow and nitrate transport in a regional or watershed scale, and incorporating uncertainties in data and information of site and contaminant.

A well as the fertilizer application that was a main management target in this study, many types of nitrogen sources are spatially distributed in the agricultural regions, such as dairy and poultry manure, dairy lagoons, atmospheric deposition, irrigation with nitrogen-contaminated groundwater, septic tanks, and nitrogen fixed by legumes. A geographic Information System (GIS) can be useful in evaluating and managing spatial information of these sources and the resulting contaminations, while the backward transport simulation was suggested in this study as a method to identify the sources influential to the wells and then to significantly manage them.

Estimation of leaching mass in the developed models did not consider any nitrogen dynamics, such as mineralization, immobilization, nitrification,
denitrification, volatilization, and plant uptake, which usually require unknown and uncertain data for material and reaction. Particularly, denitrification can be neglected because of the aerobic and oxidizing conditions of aquifer in the study area. Actually, the use of simple analytical model, which assuming constant moisture content as well as not considering nitrogen dynamics, for solute transport in unsaturated zone was also a choice to guarantee stability of optimization model by simplifying the overall simulation-optimization procedure including assessment of groundwater pumping effects. Above all, this choice was helpful in approximation of leaching to the fluctuating water table by groundwater pumping. In addition, because denitrification is a process of mass reduction of nitrate in soil and aquifer, its neglect can lead to overregulation but might provide a conservative management plan for the pursuit of safe and secure groundwater use. Nevertheless, nitrogen dynamics in unsaturated zone must be important in estimation of nitrate leaching to groundwater in the agricultural regions where have different soil conditions from this study area.

Uncertainty analysis is important for reliable prediction and management of agricultural groundwater contamination. A number of uncertainties, arising from inherent heterogeneity of geological materials, errors in field test and measurement, less well-known biogeochemical
reaction of nitrogen, changes in weather such as precipitation, and individual agricultural activities, make it difficult to understand fate of nitrate in the subsurface zone. Sensitivity analysis and stochastic approaches will be useful to account for these uncertainties.

Regional scale of agricultural contamination prediction and management are essential because the regional groundwater flow depending on characteristics of watershed bounded by mountain ridge, stream, river, and lake must be critical to the transport of nitrate in the aquifer. Seasonal precipitation is another main factor affecting groundwater level and flow in the watershed. Obviously, a number of pumping wells and nitrogen sources distributed spatially in the watershed should also be considered in this procedure using GIS. But too many decision variables, complicated groundwater flow and nitrate transport and reaction, or parameter uncertainties can prevent the optimization model from achieving the optimal solution within a reasonable time. High-performance computer, parallel computing or simplification of simulation and optimization process through grouping or classification of contaminant sources and pumping wells can be helpful in solving this problem.

Some conflicts resulting from the implementation of a specific management option might be natural in the situations that any management
option is quite difficult to satisfy all the persons concerned having competing objectives and demands. For example, a management option such as land use change or control of fertilizer application can impose a reduction in agricultural income on farmers. These conflicts related to agricultural groundwater contamination and management might sometimes lead to a social and political problem. Therefore, management options and criteria should include various potential implications in environmental, economic, social, and political aspects in order to establish more realistic and balanced management plan. Multi-criteria decision analysis such as importance order of criteria and analytic hierarchy process will be helpful in determining the reasonable management option. Also, application of an agro-economical model to assess actual cost-benefit for each management option in the variable market conditions will provide another definite basis in the decision making, while a simple economic consideration for fertilizer application and crop yield was introduced in the study. In order to reduce conflicts and to make a reasonable decision making and consensus, above all, the importance of accurate, realistic, and reliable prediction of groundwater contamination for each management option is emphasized once again.
CONCLUDING REMARKS

This study for the agricultural contaminant loading management was originated from a fundamental hydrogeolocal idea that groundwater quantity is never irrelevant to its quality. It is quite obvious that the groundwater pumping changes its level and flow and, as a result, also affects the fate of a solute such as leaching to the water table and migration in the aquifer. Therefore, in the agricultural regions where groundwater use has been common, it must be important to consider pumping conditions in the contaminant loading management as well as to determine appropriate contaminant loading mass. In the study area, effects of the fertilizer application in greenhouses on the groundwater quality in their neighboring wells were found, for example the concentrations on only those wells have fluctuated extremely and were sometimes above the water quality standard, as introduced in Chapter II. The groundwater pumping must be one of the most influential factors on the groundwater quality in this study area where a significant amount of groundwater have been used for agriculture in the large number of pumping wells. However, almost all previous studies about agricultural contaminant loading management did not consider the effects of groundwater use on the groundwater quality and manage both of the
contaminant loading and groundwater use.

In this study, the importance of considering pumping condition in determining the contaminant loading management in agricultural regions where groundwater use has been common was demonstrated and three contaminant loading management models possible to consider the pumping conditions were developed using the simulation-optimization method.

(1) In the Chapter III, the management model to determine only the optimal contaminant loading mass for a given pumping condition was first developed based on the field investigation and monitoring introduced Chapter II. Periodical on-ground contaminant loading on non-point sources such as greenhouse farming was simulated by integrating the 1-D analytical solution for solute transport in the unsaturated zone and the 3-D numerical model for groundwater flow and solute transport in the saturated zone. Backward transport simulation was applied to the model in order to sort out the influential contaminant sources for a given pumping condition and to determining the optimal contaminant loading on those sources more significantly. Genetic algorithm was linked to this integrated simulation model as optimization technique. The model can be useful in the agricultural contaminant loading management in the agricultural regions where many
potential non-point sources were located at.

(2) In the Chapter IV, using the model developed in Chapter III, the effects of pumping conditions in determining the optimal contaminant loading were quantitatively examined by comparing the optimal contaminant loading designs obtained under various pumping rates. The results demonstrated that the optimal designs were determined differently according to the given pumping rates on the wells. In addition, another management model was developed to optimize the contaminant loading mass and pumping rates simultaneously. This model cannot consider only dynamics between fate of contaminant and pumping but also various conditions such as different usage of, or demand on, each pumping well and contaminant source in a single of optimization process. The optimal design determined from this model allowed more amounts of both of contaminant loading and groundwater pumping than any other optimal design suggested previously.

(3) In the Chapter V, the model to simultaneously manage agricultural contaminant loading and groundwater use under time-variant pumping condition was also developed. For this, the method to approximate the
contaminant leaching to the fluctuating water table caused by a regular schedule of groundwater pumping was suggested and transient groundwater flow simulation was applied. In the optimal design obtained under the time-variant pumping condition, the contaminant loading was restricted significantly because a relatively large amount of contaminant leaching to the shallow depth of water table during the period without groundwater pumping, a strong inflow of the leaching contaminant to the wells driven by the large amount of pumping for a specific time of period, and a sudden increase of contaminant leaching immediately after stopping the operation of pumping. This model can be useful in determining agricultural contaminant loading in the agricultural regions where groundwater use has been concentrated in a specific time of period, such as rice-growing season, in particular like the study area.

Particularly, like some previous studies about agricultural contaminant loading which had not considered any pumping condition, the optimal design under the no-pumping condition was obtained and applied to the cases having various pumping conditions in order to demonstrate the importance of considering pumping condition in the agricultural contaminant loading. The result showed that the optimal design obtained without considering pumping condition could be failed in the agricultural
regions where groundwater is used.

The management models developed in this study can be useful in the agricultural contaminant loading management in the regions where groundwater has been commonly used for agriculture.
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국문 초록

농업지역들에서는 많은 양의 지하수가 이용되고 있는데 때때로 농업 활동으로 인해 지하수의 수질이 오염되고 있다. 따라서 농업지역에서의 지속가능한 지하수 이용을 위해서는 비료와 같은 농업오염물질의 부하를 적절히 관리하는 것이 중요하다. 하지만 지하수를 양수할 경우 지표 아래로 유입된 오염물질의 거동에 큰 영향을 미칠 수 있기 때문에 농업오염물질의 부하를 관리하고자 할 때에는 양수 조건이 고려되어야 한다.

본 연구에서는 경기도 이천시의 농촌 마을에서 수행된 현장 조사와 관측 결과를 바탕으로 주어진 양수조건 하에서 오염물질의 부하허용량을 결정하는 관리 모델을 모사-최적화 방법을 적용하여 개발하였다. 비닐하우스에서의 비료 살포 행위처럼 지표로의 주기적인 오염물질의 부하를 모사하기 위해 1차원의 불포화대 내 용질 거동에 관한 해석과 3차원의 지하수 흐름 및 포화대 내 용질 거동에 관한 수치 모델을 결합하였다. 또한 많은 오염원들 중 실제 관정 오염에 영향력있는 오염원을 구분하고 그들에게 보다 중요하게 관리가 이루어질 수 있도록 역산 거동 모델이 적용되었다. 유전자 알고리즘은 최적화 기법으로서 앞서 설명된 모사 모델과 연동된다. 개발된 모델은 오염원이 많이 분포한 지역에서 농업오염물질의 부하를 관리하고자 할 때 유용할 것으로 판단된다. 본 모델을 이
용하여 여러 양수 조건하에서 얻은 최적 부하허용량 설계를 서로 비교함
으로써 양수 조건이 부하허용량 설계에 미칠 수 있는 영향에 대해 살펴
보았다. 결과는 부하허용량 설계가 주어진 양수 조건에 따라 다르게 결
정될 수 있음을 보였다. 본 연구에서는 부하허용량과 양수량을 동시에
설계할 수 있는 또 다른 관리모델이 개발되었다. 이는 양수와 오염물질
의 거동 간의 복잡한 역학관계나 양수정 및 오염원들에 대한 요구량 혹
은 사용량 등의 다양한 조건을 반영할 수 있다는 장점이 있다. 무엇보다
이 모델로부터 결정된 최적 설계는 앞서의 어떤 설계들보다도 더 많은
양수량과 부하량을 허용하도록 하고 있었다. 또한 벼의 생장기간 동안
많은 양의 지하수가 이용되는 것처럼, 지하수가 특정 기간 동안 집중적
으로 이용되는 농업지역들의 경우 농업오염물질의 부하허용량을 결정함
에 있어 그러한 양수 조건을 고려하는 것이 특히 중요할 것이다. 이에
시기에 따라 변하는 양수 조건 하에서 부하허용량과 양수량을 동시에 관
리할 수 있는 모델이 개발되었다. 이를 위해 특정 기간의 양수로 인해
변동하는 지하수면으로의 오염물질의 침출을 근사하는 방법이 모색되었
으며, 부정류 지하수 흐름 모델링이 적용되었다. 시기에 따른 양수 조건
하에서는 앞서의 결과들에 비해 오염 부하가 상당히 제한되었는데, 이는
양수가 없는 시기 동안 얻은 지하수면으로 많은 양의 침출이 있었고 양
수가 있는 시기 동안엔 양수로 인해 관점으로 오염운의 유입이 발생하였.
으며, 양수가 끝난 직후 상승하는 지하수면으로 지표로부터 부하된 오염물질이 일시에 침출하였기 때문에 쓰고 있으므로 판단하고 있다. 특히 본 연구에서 보인 양수가 없는 조건 하에서의 최적 설계 결과는 농업지역의 오염물질 부하 관리에 있어 양수 조건 고려의 중요성을 보이기 위해서 수행한 것으로, 양수 조건을 고려하지 않은 채 농업지역에서의 오염물질 부하를 관리하고자 하였던 연구들을 그대로 따라한 것이다. 그 결과는 지하수의 이용이 흔한 농업지역에서 양수를 고려하지 않고 오염물질의 부하를 관리할 경우 실패할 수 있다는 것을 지적하고 있다.

주요어: 농업 오염물질 부하 관리; 질산성질소; 비닐하우스 내 비료 살포; 모사-최적화 모델; 지하수 양수; 지하수면 변동; 오염부하허용량.