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Spreadsheet Models for Determining the Influence of Land Applications of Fertilizer on Underlying Groundwater Nitrate Concentrations

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Spreadsheet Models for Determining the Influence of Land Applications of Fertilizer on Underlying Groundwater Nitrate Concentrations

by

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Abstract

Groundwater quality characterization studies have identified significant regional-scale problems with nitrate contamination across Washington State. This contamination is often found in close association with nonpoint applications of nitrogen-bearing fertilizers or animal manure to agricultural lands. Due to the risk that nitrate poses to state drinking water supplies, determining the proper balance between nutrient application rates, crop uptake, and nitrate loss to groundwater is a growing priority in Washington.

This report presents a set of three spreadsheet computer models that can be used to quantitatively predict the impact of residual or excess farm-field soil nitrate on the concentration of nitrate in underlying shallow groundwater.

- Model 1 (NO₃-LEACHATE) is a mixing model used to predict the dissolved nitrate concentration that results when a known volume of recharge infiltrates and fully mixes with a residual mass of nitrate present in vadose-zone soils.
- Model 2 (GWNO₃-FORECAST) is a mass balance mixing model used to predict the groundwater nitrate concentration that will result when the nitrate-bearing leachate predicted by Model 1 enters an aquifer and mixes with ambient groundwater flowing beneath the site of application.
- Model 3 (GWNO₃-BACKCAST) uses modified versions of the Model 1 and 2 equations to back-calculate the nitrate concentration in vadose-zone leachate, the nitrate mass load, and the average shallow soil nitrate concentration required to maintain a given concentration of nitrate in underlying groundwater.

All three models allow the user flexibility in defining site-specific model variables, including the subsurface hydrologic properties of the site, estimates of soil nitrate concentration and bulk density, and nitrate attenuation processes active in both the vadose and saturated zones. Model assumptions and limitations are discussed.

The purpose of this publication is to provide guidance to users of these models.

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Introduction

Contamination of groundwater with dissolved nitrate (NO_3^- ; a highly soluble anion containing nitrogen) is a widespread problem in Washington State. Groundwater quality characterization studies have identified significant regional-scale problems with nitrate, including aquifer systems in the central Columbia Basin, the Yakima Basin, and Whatcom County (Ryker and Frans, 2000; Sell and Knutson, 2002; USEPA, 2013; Carey and Cummings, 2012). Wells sampled during these studies have shown dissolved nitrate concentrations frequently above (failing) the Washington State groundwater quality standard of 10 milligrams per liter (mg/L) nitrate as nitrogen (nitrate-N or $\text{NO}_3\text{-N}$)(Chapter 173-200 WAC).

Although nitrate can be derived from a variety of natural and anthropogenic sources, nonpoint applications or releases of nitrogen-bearing fertilizers and animal manure to agricultural lands represent the largest sources of nitrate mass released to the environment (Puckett, 1994; Viers et al., 2012). In several areas of concern in Washington, nitrogen fertilizer¹ applications to agricultural lands have been identified as the primary known or likely source of nitrate contamination in groundwater (Frans, 2000; Carey and Cummings, 2012; USEPA, 2013; Carey and Harrison, 2014). As a result, the proper management and control of nitrogen related to agricultural activities is becoming a subject of increasing focus for the Washington State Department of Ecology and for the agricultural industry at large.

Due to its high solubility, nitrate present in a soil column in amounts that exceed crop demand can be rapidly mobilized into solution by downward infiltrating recharge derived from precipitation, irrigation, or both. When the resulting nitrate-enriched leachate moves below the base of the crop root zone, the nutrients are no longer available for plant uptake. If this leachate continues to move downward through the vadose zone and reaches the water table, it can pose a significant risk to the quality of the underlying groundwater. Due to this risk, determining the proper balance between nutrient application rates, crop uptake, and nitrate loss to groundwater is a growing priority in Washington.

This report documents a set of three mathematical models that can be used to quantitatively predict the influence of residual or excess farm-field soil nitrate on the concentration of nitrate in underlying groundwater. The models are based on adaptations of standard mixing and mass-balance principles that have been used to examine contaminant loading to groundwater for many decades (e.g., Summers et al., 1980; Wehrmann, 1984; Bauman and Shafer, 1985; USEPA, 1996; Taylor, 2003; Viers et al., 2012). The models have been incorporated into an interactive Microsoft Excel 2007[®] spreadsheet file issued with this report.

The tools described in this report are intended to be used to:

- Assist decision-making about nitrogen fertilizer application rates at the field scale.
- Improve the user's understanding of the potential consequences to underlying groundwater quality when land-applying nitrogen-enriched fertilizer in excess of crop demand.

¹ The term *fertilizer* includes both inorganic and organic (manure-based) forms.

- Identify the factors that play the most significant role in nitrate loading impacts to groundwater systems.
- Compare the relative potential for nitrate groundwater contamination between sites.

The models presented in this report allow the user to specify the values for many of the equation terms; this flexibility makes it possible to generate predictions using site-specific conditions. Model assumptions and limitations are presented for each model to guide the user in deciding appropriate use and in assigning appropriate uncertainty to the predictions. Model users are expected to have a working understanding of the sciences of hydrogeology and nitrogen cycling.

Model 1 - NO3-LEACHATE

NO3-LEACHATE Model Description

The NO3-LEACHATE model assumes that all recharge² reaching the water table during a model scenario period of interest dissolves (fully mixes with) all residual nitrate mass present in the vadose zone³ beneath the modeled field. The model calculates the dissolved nitrate-N concentration of the resulting leachate arriving at the water table. The model can accommodate ten independent model scenarios.

Estimates of the residual nitrate-N mass available to leach can be derived from either: (A) near-surface soil nitrate-N sampling results, or (B) a farm-field nitrogen mass balance analysis. Any dissolved nitrate-N present in the recharge prior to its infiltration into the subsurface is accounted for in the final leachate concentration prediction. The model can also account for any nitrate concentration decrease that occurs in the leachate due to attenuation processes active during mixing and transport within the vadose zone.

A schematic of the conceptual model for Model 1 is shown in Figure 1. Variable symbols shown on the figure are explained in detail below. The predicted Model 1 leachate concentration value for each model scenario is automatically carried forward for use as an input variable in the corresponding Model 2 scenario (GWNO3-FORECAST; described later in this report).

² For this report, recharge is defined as the water volume that infiltrates through the vadose zone, reaches the water table, and adds to groundwater storage by the end of the model scenario period of interest. Recharge can be derived from the infiltration of precipitation, or from irrigation, or from a combination of the two.

³ For this report, the *vadose zone* is defined as the zone between the land surface and the regional water table, including the soil column.

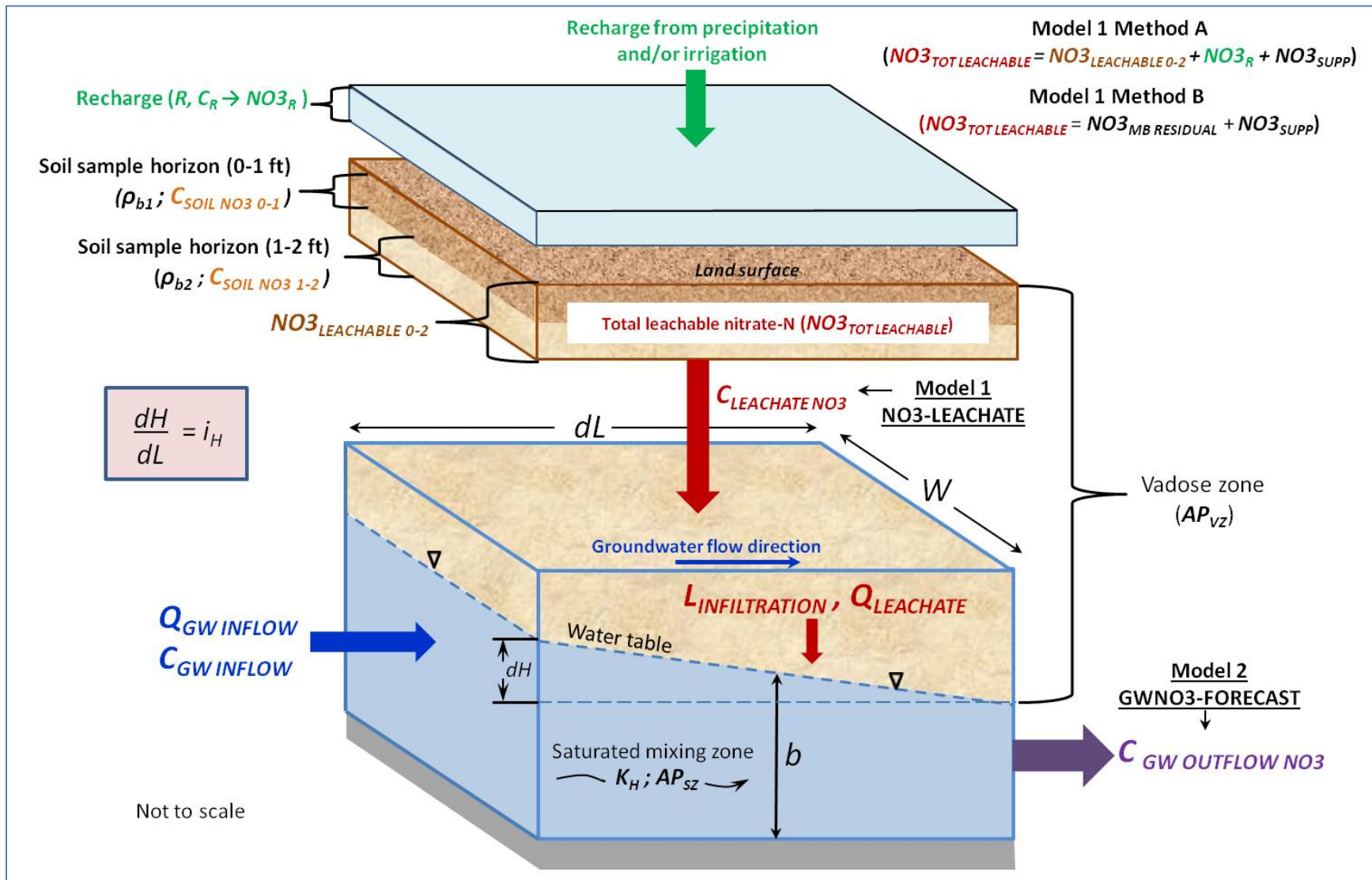


Figure 1. Conceptual Model Schematic – Models 1 (NO3-LEACHATE) and 2 (GWNO3-FORECAST). Refer to text for further explanation of figure symbols.

In the NO₃-LEACHATE model, two different approaches can be used to estimate the amount of residual nitrate-N available for dissolution:

NO₃-LEACHATE, Method A

In Method A, the mass of residual nitrate-N available to leach to groundwater from the upper soil column is calculated using soil nitrate-N sample concentration data (or estimates) from the 0-1 and 1-2 foot soil horizons ($C_{SOIL\ NO_3\ 0-1}$ and $C_{SOIL\ NO_3\ 1-2}$). It is a common agronomic practice on fertilized fields to collect soil nitrate-N samples from the uppermost portion of the soil column at the end of the growing season (see for example Sullivan and Cogger, 2003; Ehrhardt and Bundy, 1995; Camberato et al., 2013; Dinkins and Jones, 2007; Carey, 2002; Carey and Harrison, 2014). This type of field data therefore provides a readily available basis for estimating leachable soil nitrate mass.

The total leachable soil nitrate-N mass estimate for the top two feet of the soil column ($NO_{3LEACHABLE\ 0-2}$) is determined by first converting the average measured (or assumed) soil nitrate *concentration* value to an equivalent nitrate-N unit area *mass* for each horizon, and then summing these two mass values. Soil bulk density values assigned to each horizon by the user ($\rho_{b\ 0-1}$ and $\rho_{b\ 1-2}$) are factored into the concentration-to-mass conversion.

In addition to the $NO_{3LEACHABLE\ 0-2}$ mass, the Method A model can, if appropriate, also account for two additional sources of nitrate-N mass not accounted for by the $NO_{3LEACHABLE\ 0-2}$ term:

- The nitrate-N mass contributed by the recharge itself (NO_{3R}). To determine the NO_{3R} value, the user provides (1) the estimated nitrate-N concentration of the recharge *prior to its entry* into the vadose zone ($C_{R\ NO_3}$) and (2) the total volume of recharge (R) estimated to reach the water table by the end of the scenario period of interest. For each scenario, the model then combines these values to calculate the mass of nitrate-N supplied by infiltrating precipitation and/or irrigation water.
- A mass of vadose-zone nitrate-N that mixes with the infiltrating recharge that is *supplemental to* the $NO_{3LEACHABLE\ 0-2}$ value (NO_{3SUPP}). This variable allows the user to account for soluble nitrate-N that is (or becomes) available to leach during each model scenario period of interest that is *not otherwise* accounted for by the $NO_{3LEACHABLE\ 0-2}$ value. Example nitrate sources the NO_{3SUPP} variable could represent include:
 - Leachable nitrate-N mass present in the vadose zone below 2 feet.
 - Nitrate-N mass leached *prior* to soil nitrate sampling (but still within the scenario period of interest).
 - Nitrate-N mass produced by continued microbial conversion of organic nitrogen to nitrate (by mineralization/nitrification), occurring after soil nitrate sample collection, but still within the scenario period of interest. (Norton, 2008; UCD, 2009).

The three distinct sources of soluble nitrate-N mass ($NO_{3LEACHABLE\ 0-2}$, NO_{3R} , and NO_{3SUPP}) are summed to determine the total nitrate-N mass available to leach to groundwater per acre ($NO_{3TOT\ LEACHABLE}$).

NO3-LEACHATE, Method B

In place of soil sampling results, this method uses the residual from a mass balance evaluation of nitrogen inputs and outputs to a farm field ($N_{MB\ RESIDUAL}$) to estimate the mass of soluble nitrate-N available for leaching per acre. It is assumed that the *nitrogen* mass residual estimated by the mass balance is fully converted to *nitrate* and is therefore equivalent to the mass of soluble nitrate-N available for leaching within the scenario period of interest (i.e., $N_{MB\ RESIDUAL} = NO3_{MB\ RESIDUAL}$).

Similar to Method A, Method B also allows the user to assign an additional mass contribution from supplemental sources of nitrate-N ($NO3_{SUPP}$) for any reason not otherwise accounted for by the mass balance analysis, if appropriate. The nitrate-N contribution from recharge is assumed to already be accounted for in the mass balance input-output evaluation and is therefore not included as a separate, explicit variable in the Method B equations.

The two distinct sources of soluble nitrate-N mass estimated for Method B ($NO3_{MB\ Residual}$ and $NO3_{SUPP}$) are summed to determine the total nitrate-N mass available to leach to groundwater per acre ($NO3_{TOT\ LEACHABLE}$).

NO3-LEACHATE, Methods A and B

Once a $NO3_{TOT\ LEACHABLE}$ mass value has been determined for a model scenario (using either Method A or B above), the value is combined with the scenario period-of-interest recharge estimate (R) to calculate the nitrate concentration of the leachate reaching the water table. Before predicting the final leachate concentration, the NO3-LEACHATE model allows the user to also account for any vadose-zone processes (such as denitrification) that act to decrease the nitrate concentration of the leachate during mixing and transport. This is accomplished by applying a term, *vadose-zone attenuation percentage* (AP_{VZ}), in the final model calculation.

Method A and/or B model predictions of the nitrate-N concentration of the leachate are automatically graphed for each model scenario by the accompanying Excel 2007[®] worksheet (Figure 2).

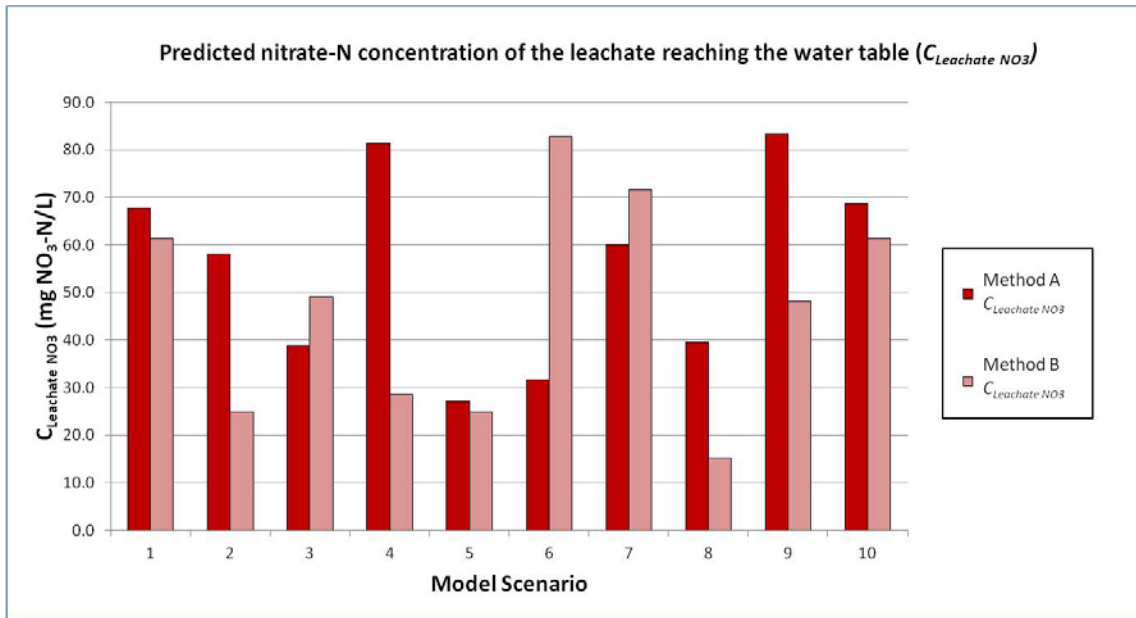


Figure 2. Example output graph from the NO3-LEACHATE model spreadsheet.

NO3-LEACHATE Model Equations

If using Method A

Near-surface soil nitrate-N sample concentration data can be used to estimate the mass of leachable nitrate-N in the top 2 feet of the soil column for each model scenario using Equation 1:

$$NO3_{LEACHABLE\ 0-2} = NO3_{LEACHABLE\ 0-1} + NO3_{LEACHABLE\ 1-2} \quad \text{Eq. 1}$$

where: $NO3_{LEACHABLE\ 0-1} = 2.719(\rho_{b\ 0-1} * C_{SOIL\ NO3\ 0-1})$ Eq. 2

and: $NO3_{LEACHABLE\ 1-2} = 2.719(\rho_{b\ 1-2} * C_{SOIL\ NO3\ 1-2})$ Eq. 3

where:

$NO3_{LEACHABLE\ 0-2}$ = leachable nitrate-N mass present in the 0-2 foot soil horizon (lbs NO₃-N/acre).

$NO3_{LEACHABLE\ 0-1}$ = leachable nitrate-N mass present in the 0-1 foot soil horizon (lbs NO₃-N/acre).

$NO3_{LEACHABLE\ 1-2}$ = leachable nitrate-N mass present in the 1-2 foot soil horizon (lbs NO₃-N/acre).

$\rho_{b\ 0-1}$ = average soil bulk density, 0-1 ft soil horizon (g/cm³).

$C_{SOIL\ NO3\ 0-1}$ = average dry-weight soil nitrate-N concentration in the 0-1 foot soil horizon (mg NO₃-N/Kg DW).

$\rho_{b\ 1-2}$ = average soil bulk density, 1-2 ft soil horizon (g/cm³).

$C_{SOIL\ NO_3\ 1-2}$ = average dry-weight soil nitrate-N concentration in the 1-2 foot soil horizon (mg NO₃-N/Kg DW).

The total mass of nitrate-N that is available to leach to groundwater is calculated as follows:

$$NO_3_{TOT\ LEACHABLE} = NO_3_{LEACHABLE\ 0-2} + NO_3_R + NO_3_{SUPP} \quad \text{Eq. 4}$$

where: $NO_3_R = 2.719(R * C_{R\ NO_3})$ Eq. 5

where:

$NO_3_{TOT\ LEACHABLE}$ = total nitrate-N mass available to leach to groundwater (lbs NO₃-N/acre).

NO_3_R = mass of soluble nitrate-N contributed to the leachate by recharge (lbs NO₃-N/acre).

NO_3_{SUPP} = supplemental nitrate-N mass contributed to the leachate that is *not otherwise* accounted for by the $NO_3_{LEACHABLE\ 0-2}$ or NO_3_R values (lbs NO₃-N/acre).

R = amount of recharge reaching the water table during the scenario period of interest (ft).

$C_{R\ NO_3}$ = nitrate-N concentration in recharge (precipitation and/or irrigation water) *prior to* infiltration (mg NO₃-N/L).

If using Method B

Users relying on a farm-field mass balance approach can calculate $NO_3_{TOT\ LEACHABLE}$ for each model scenario using a mass balance residual value in the following manner:

$$NO_3_{TOT\ LEACHABLE} = NO_3_{MB\ RESIDUAL} + NO_3_{SUPP} \quad \text{Eq. 6}$$

assuming: $NO_3_{MB\ RESIDUAL} = N_{MB\ RESIDUAL} = N_{INPUTS} - N_{OUTPUTS}$ Eq. 7

where:

$NO_3_{MB\ RESIDUAL}$ = the residual nitrate-N mass determined from a mass balance analysis of nitrogen inputs and outputs to the model area (lbs NO₃-N/acre).

NO_3_{SUPP} = supplemental nitrate-N mass contributed to the leachate that is *not otherwise* accounted for by the mass balance analysis (lbs NO₃-N/acre).

$N_{MB\ RESIDUAL}$ = farm-field mass balance nitrogen residual (lbs-N/acre).

N_{INPUTS} = sum of total nitrogen inputs to the model area (lbs-N/acre).

$N_{OUTPUTS}$ = sum of total nitrogen outputs from the model area (lbs-N/acre).

Method A and B

Once a $NO_3_{TOT\ LEACHABLE}$ value has been determined, the nitrate-N concentration of the leachate reaching the water table ($C_{LEACHATE\ NO_3}$ on Figure 1) can be estimated for each model scenario using a modified version of an equation presented by Carey and Harrison (2014):

$$C_{LEACHATE\ NO3} = \frac{NO3_{TOT\ LEACHABLE}}{2.719R} * (1 - \frac{AP_{VZ}}{100}) \quad \text{Eq. 8}$$

where:

$C_{LEACHATE\ NO3}$ = nitrate-N concentration of the leachate that reaches the water table (mg NO₃-N/L).

AP_{VZ} = vadose-zone attenuation percentage; percent nitrate-N concentration decrease that occurs in the leachate during transport through the vadose zone, due to denitrification or other attenuation processes (0% to 100%).

See Appendix A for the derivation of the conversion factors used in the above equations.

NO₃-LEACHATE Model Assumptions

The model calculations assume the following conditions for each scenario:

- The model predictions represent the condition at the end of the scenario period of interest.
- The soil properties $C_{SOIL\ NO3\ 0-1}$, $C_{SOIL\ NO3\ 1-2}$, $\rho_b\ 0-1$, and $\rho_b\ 1-2$ are spatially uniform throughout the model area and depth-intervals of interest.
- The vadose zone is isotropic and homogeneous throughout the model area; vadose-zone attenuation effects on leachate concentrations act equally throughout the vadose-zone volume of interest, and downward flow is uniform.
- The full volume of recharge reaches the water table by the end of the scenario period of interest.
- The concentration of nitrate-N in soil determined using standard laboratory analysis techniques (e.g., 2.0N KCL extraction/ cadmium reduction method; Galvak et al., 2005) is assumed to be equivalent to the concentration of nitrate-N available to leach via recharge infiltration (Horneck, 2014).
- The leachable nitrate-N mass estimated for each scenario is fully dissolved in, and fully mixes with, the infiltrating recharge by the end of the scenario period of interest.
- Dissolved nitrate is unaffected by adsorption within the vadose zone (i.e., the sorption distribution coefficient (K_d) for nitrate is assumed to be 0 ml/g).
- For leachate predictions based on farm-field mass balance nitrogen residuals, it is assumed that the residual nitrogen will entirely convert to soluble nitrate-N within the scenario period of interest, and that nitrate-N mass contributions from recharge are already accounted for in the $NO3_{MB\ RESIDUAL}$ value. The model does not account for errors or uncertainty in the nitrogen mass balance analysis itself.
- Model scenarios are treated independently of one another and are not necessarily connected in time. Model scenarios do not inherit the adjacent scenario's input-variable values; instead, initial conditions for each scenario must be set by the user.

NO3-LEACHATE Model User-Defined Variables

The following variables can be defined by the user for each scenario in the NO3-LEACHATE model:

- $\rho_b 0-1$ and $\rho_b 1-2$ – these values may be derived from site-specific field testing. Alternatively, Appendix B presents soil bulk density ranges, broken down by soil texture class and depth-interval (0-1' and 1-2'), for both eastern and western Washington soils used for cropland. These ranges were derived from analyses of information in the U.S. Department of Agriculture's Natural Resources Conservation Service (NRCS) SSURGO database (Campbell, 2014).

Spreadsheets of the raw SSURGO data that were compiled for the analysis (including the NRCS soil map unit) are available as supplemental files to this report. Model users who have knowledge of the specific soil survey map unit(s) at their site (see the NRCS Web Soil Survey website at: <http://websoilsurvey.nrcs.usda.gov/>) may use this information to support site-specific soil bulk density determinations.

- $C_{SOIL\ NO3\ 0-1}$ and $C_{SOIL\ NO3\ 1-2}$ – if using Method A, these values are ideally derived from site-specific soil sampling results. The values should represent the average soil nitrate-N concentration for each depth horizon, across the entire area of interest being modeled (see for example standard soil nitrate sample collection procedures described by Sullivan and Cogger, 2003). In some areas, soil nitrate sampling is only conducted for the top one foot of the soil column. Users in this case can enter an assumed concentration value for the $C_{SOIL\ NO3\ 1-2}$ term. If this term is ignored (i.e., set to a value of 0 mg/Kg), any soil nitrate present in the 1-2 foot horizon will be ignored in the model calculations.
- $NO3_{SUPP}$ – if a site-specific value for this variable is unavailable, a default value of 0 lbs/acre is recommended for the initial model run. In some cases, this value may only be estimated through an inverse calibration process with Model 2 (described below). The resulting $NO3_{SUPP}$ value may generically represent nitrate-N loading from a source or sources that are otherwise difficult to accurately quantify in the field (e.g., post-sampling mineralization/nitrification).
- R – this value should preferably be derived from a site-specific analysis of recharge. The value should represent the total amount of recharge, from all sources (precipitation and/or irrigation) estimated to reach the water table by the end of the model scenario period of interest. Healy (2010) provides in-depth discussion of the methods available to estimate recharge. If an annual rate of recharge is used to determine an R value for a model scenario that represents less than a full year, R should be decreased accordingly (and seasonal variability should be accounted for). Users should also be sure that the chosen value for R is reasonably consistent with the model assumptions regarding complete mixing and dissolution. For example, even if the recharge value set by the user for the scenario is very small, the model will nonetheless assume that that water volume will completely mix and flush the designated leachable nitrate-N mass. Although this is an unlikely occurrence in the field, the model will nonetheless proceed with the calculations, resulting in an unrealistically high $C_{LEACHATE\ NO3}$ prediction.

- C_{RNO3} – for recharge derived solely from precipitation, a recommended value for this variable for sites located east of the Cascade Mountains is 0.09 mg NO₃-N/L. West of the Cascades, a value of 0.05 mg NO₃-N/L is suggested (see Appendix C). If recharge is partly or wholly derived from irrigation, the nitrate-N concentration of the irrigation water prior to application should be measured and accounted for in the C_{RNO3} value.
- $NO3_{MB\ Residual}$ – if using Method B, this value should be derived from a site-specific mass balance analysis of farm-field nitrogen inputs and outputs. If the model user has evidence to suggest that only a portion of the total nitrogen residual identified by the mass balance analysis converts to soluble nitrate (i.e., $N_{MB\ RESIDUAL} \neq NO3_{MB\ RESIDUAL}$), the user should adjust the model input value for $NO3_{MB\ RESIDUAL}$ accordingly (see UCD, 2009 and Sullivan, 2008 for additional discussion). If the mass balance nitrogen residual is a negative value, a value of zero (0) should be entered into the model for this variable.
- AP_{VZ} – if a site-specific value for this variable is unavailable, a default value of 0% is recommended for the initial model run (i.e., conservative transport). Model users should note that field research has indicated that concentration reductions of dissolved nitrate-N during transport between the base of a root zone and the capillary fringe of the water table can be very limited in many settings. When this does occur, it can be a highly localized phenomenon (Green et al., 2008; Onsoy et al., 2005; Artiola, 1997). Holden and Fierer (2005) also note the tendency for denitrification rates to drop off rapidly with depth in the vadose zone. Users setting the AP_{VZ} value above ~10% should have compelling field information to justify the higher value.

NO3-LEACHATE Model Limitations

The NO3-LEACHATE model greatly simplifies the highly complex nature of chemical dissolution and transport observed in many vadose-zone settings. For example:

- Time is not explicitly accounted for in the NO3-LEACHATE model equations; the mixing of recharge with the leachable nitrate mass present within the vadose zone, and the transport of the resulting solution to the water table, is simply assumed to be complete by the end of each model scenario. When interpreting the model results, users should keep in mind any special field conditions at their site that may differ significantly from this assumption (e.g., long-term storage of infiltration in the vadose zone, a deep water table, or delays in downward infiltration due to permeability contrasts).
- The model assumption that the designated recharge volume will fully mix with and dissolve all of the nitrate-N mass present in the soil column within the scenario period of interest ignores the potential influence of spatial heterogeneity, anisotropy, and preferential (non-uniform) flow. In the field, however, these factors can cause large variations in the extent, timing, and rate of nitrate dissolution and transport (see, for example, Sebilo et al., 2013; Onsoy et al., 2005).
- The model ignores any processes occurring during the scenario period of interest such as plant uptake of soil nitrate that may reduce the amount of nitrate mass that is available to leach. This suggests that the NO3-LEACHATE model is best used for examining nitrate leaching outside of the active growing season.

- The accuracies of the NO₃-LEACHATE model predictions are a function of uncertainties or errors in the leachable nitrate mass estimates derived by soil sampling (Method A) or farm-field mass balance analysis (Methods B). For example, Carey and Harrison (2014) demonstrated that the timing of soil nitrate sample collection can be a critical factor when attempting to evaluate the amount of soil nitrate available for leaching to groundwater. These authors showed that mineralization processes active subsequent to soil sampling may produce leachable soil nitrate mass not accounted for by the sample results. Shallow soil sampling may also fail to measure nitrate mass that has moved deeper into the vadose zone. Similarly, nitrogen mass balance analysis methods normally rely on assumptions about complex nitrogen cycle processes, such as mineralization or volatilization rates, that may not accurately reflect the modeled site.

Failure to account for all components of the nitrogen cycle, or errors in the measurement or estimation of those components, can impact the accuracy of the residual nitrate mass estimates required by the NO₃-LEACHATE model (in turn, influencing the accuracy of the $C_{LEACHATE\ NO_3}$ predictions).

Assuming the estimate(s) of total leachable nitrate accurately reflects the nitrate mass actually present in the subsurface at the modeled site, the assumption of *complete* dissolution and transport of that mass may tend to overestimate the amount of nitrate mass reaching the water table during a scenario. In that case, the model predictions of the leachate concentration should be considered conservative (upper-bound) estimates. However, if the nitrate mass available to leach within the model domain is underestimated, the leachate concentration predictions may be lower than what actually occurs in the field.

Model 2 - GWNO3-FORECAST

GWNO3-FORECAST Model Description

The GWNO3-FORECAST model estimates the nitrate-N groundwater concentration that will result after a nitrate-enriched leachate enters an aquifer from the overlying vadose zone and mixes with ambient groundwater flowing beneath an application site.

In this mass-balance box model, based on principles described by Summers et al. (1980), leachate arriving at the water table with a nitrate concentration $C_{LEACHATE\ NO3}$ enters a saturated mixing zone of interest with a user-defined average thickness b (see Figure 1). The leachate fully mixes with groundwater that is entering the upgradient boundary of the mixing zone with a nitrate concentration of $C_{GW\ INFLOW\ NO3}$ at a rate of $Q_{GW\ INFLOW}$.

The model predicts the steady-state nitrate-N concentration of the resulting groundwater/leachate mix that exits the downgradient boundary of the model domain ($C_{GW\ OUTFLOW\ NO3}$). If appropriate, the user can account for processes that act to decrease the groundwater nitrate-N concentration during mixing and transport (for example, saturated-zone denitrification). This is accomplished by applying a term called the saturated-zone attenuation percentage (AP_{SZ}) in the final model calculation. The AP_{SZ} variable is intended to represent attenuation processes that are *distinct from* those that occur within the vadose zone.

To calculate the $C_{GW\ OUTFLOW\ NO3}$ value, the GWNO3-FORECAST model uses a $C_{LEACHATE\ NO3}$ concentration value carried forward from the corresponding scenario from the NO3-LEACHATE model. The GWNO3-FORECAST predictions for $C_{GW\ OUTFLOW\ NO3}$ are automatically graphed by the spreadsheet for a maximum of ten independent model scenarios.

In the accompanying spreadsheet file, the user can also enter measured concentrations of nitrate-N in groundwater for each period to determine how well the model predictions align with field-based data (Figure 3). If appropriate, the model can be calibrated to the field data by adjusting the user-designated values; this calibration process *can include modification of the Model 1 inputs*. If the model is calibrated using this inverse approach, input values should only be adjusted within a range deemed suitable for the site conditions, or consistent with results from previous research.

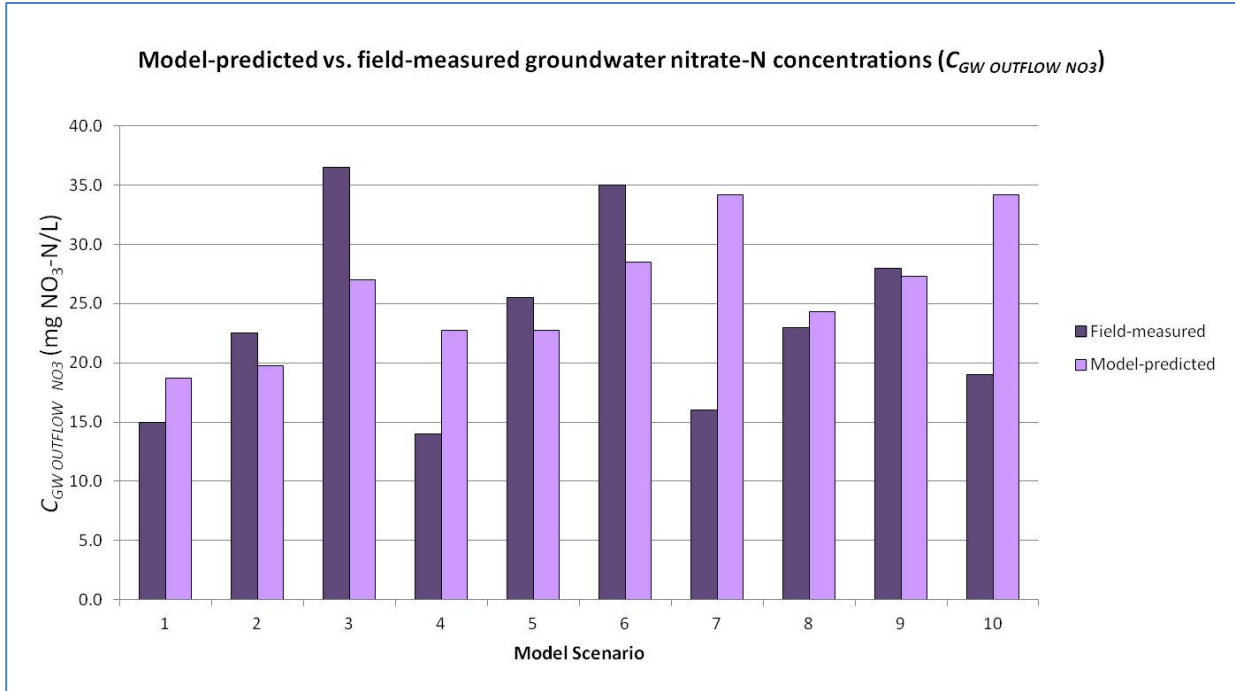


Figure 3. Example output graph from the GWNO3-FORECAST model spreadsheet.

GWNO3-FORECAST Model Equations

Equation 9, modified from Summers et al. (1980) and KGS (1994), is used to estimate the groundwater nitrate-N concentration resulting from the infiltration and mixing of a nitrate-enriched leachate into an underlying saturated zone:

$$C_{GW\ OUTFLOW\ NO3} = \frac{(Q_{LEACHATE} \times C_{LEACHATE\ NO3}) + (Q_{GW\ INFLOW} \times C_{GW\ INFLOW\ NO3})}{Q_{LEACHATE} + Q_{GW\ INFLOW}} * \left(1 - \frac{AP_{SZ}}{100}\right)$$

Eq. 9

where, for each model scenario:

$C_{GW\ OUTFLOW\ NO3}$ = steady-state groundwater nitrate-N concentration exiting the downgradient boundary of the saturated mixing zone at the end of the scenario period of interest (mg NO₃-N/L).

$Q_{LEACHATE}$ = volumetric flow rate of leachate entering the saturated mixing zone from the vadose zone (L/day).

$Q_{GW\ INFLOW}$ = volumetric flow rate of groundwater inflow entering the upgradient boundary of the saturated mixing zone (L/day).

$C_{GW\ INFLOW\ NO3}$ = concentration of nitrate-N in upgradient groundwater inflow *prior to* entering the saturated mixing zone (mg NO₃-N/L).

AP_{SZ} = saturated zone attenuation percentage; percent nitrate-N concentration decrease that occurs in the groundwater/leachate mix during transport through the saturated mixing zone, due to denitrification or other attenuation processes (0% to 100%);

where:
$$Q_{LEACHATE} = 28.32(dL * W * L_{INFILTRATION}) \quad \text{Eq. 10}$$

and:
$$Q_{GW INFLOW} = 28.32(K_H * b * W * i_H) \quad \text{Eq. 11}$$

where:
$$i_H = \left(\frac{dH}{dL} \right) \quad \text{Eq. 12}$$

where:

dL = length of the modeled study area, parallel to the groundwater flow direction (ft).

W = horizontal width of the modeled study area, perpendicular to the groundwater flow direction (ft).

$L_{INFILTRATION}$ = infiltration rate of recharge-derived leachate into the saturated mixing zone (ft/day).

K_H = bulk horizontal hydraulic conductivity of the mixing zone aquifer material (ft/day).

b = average thickness of the saturated mixing zone of interest (ft).

i_H = horizontal hydraulic gradient across the modeled study area (ft/ft).

dH = decrease in hydraulic head over the distance dL (ft; entered as a *positive* value).

See Appendix A for the derivation of the conversion factors used in the above equations.

GWNO3-FORECAST Model Assumptions

The GWNO3-FORECAST model calculations assume the following conditions for each model scenario:

- The model predictions for $C_{GWOUTFLOW NO3}$ represent a steady-state condition at the end of the scenario period of interest.
- The saturated zone of interest is unconfined.
- The saturated zone of interest is isotropic and homogeneous; therefore, mixing and attenuation effects on groundwater concentrations act uniformly throughout the mixing zone. The user-assigned saturated zone attenuation is complete by the end of the scenario period of interest.
- In the accompanying spreadsheet model file, the predicted values for $C_{LEACHATE NO3}$ are automatically carried forward from Model 1 (NO3-LEACHATE) to the corresponding Model 2 scenarios. The spreadsheet requires the model user to choose either the Model 1 Method A or Method B $C_{LEACHATE NO3}$ values.
- The leachate entering the mixing zone fully mixes with the groundwater estimated to enter the upgradient boundary of the model during that scenario.

- Dissolved nitrate transport through the saturated zone is unaffected by adsorption reactions (i.e., the nitrate sorption distribution coefficient (K_d) is assumed to be 0 ml/g).
- Model scenarios are treated independently of one another and are not necessarily connected in time. Therefore, scenarios do not inherit the adjacent scenario's input-variable values. Initial conditions for each scenario must be set by the user.

GWNO3-FORECAST User-Defined Variables

The following variables can be defined by the user for each scenario in the GWNO3-FORECAST model:

- $C_{LEACHATE\ NO3}$ – In the accompanying spreadsheet model file, the value for this variable is automatically carried forward from the corresponding NO3-LEACHATE model scenario⁴; the user can choose either the Method A or Method B predictions for this purpose.

If the GWNO3-FORECAST predictions for $C_{GW\ OUTFLOW\ NO3}$ are not in sufficiently close agreement with the concentrations measured in groundwater at the site, the user may consider adjusting some or all of the assigned Model 1 or Model 2 input values to improve the Model 2 calibration. For example, model predictions for $C_{GW\ OUTFLOW\ NO3}$ that are significantly below field measurements of groundwater nitrate concentration suggest that more nitrate mass may be reaching the aquifer than initially predicted. Possible calibration responses to this situation include increasing the $NO3_{SUPP}$ value in Model 1, or decreasing the attenuation percentages used in either Model 1 or Model 2. As mentioned earlier, input values should be modified only within the range deemed suitable for the site conditions, or consistent with results from previous research.

- dL and W – These horizontal dimensions of the modeled area of interest (parallel and perpendicular to the average groundwater flow direction, respectively) can be set by the user to match the measured dimensions of the study site, or for conceptual analyses, can be set to correspond to a square the size of an acre (208.7 ft * 208.7 ft).
- $L_{INFILTRATION}$ – The infiltration rate is best derived from a site-specific analysis of recharge. One method of determining the infiltration rate involves dividing the Model 1 value established for R by the estimated number of days required to accumulate that recharge amount. For example, if a 90-day water table fluctuation analysis was used to determine a value of R of 1.89 feet, the average rate of infiltration can be estimated as: 1.89 ft/90 days = 0.021 ft/day. If an annual rate of recharge is used to determine a daily infiltration rate for a scenario, users should adjust the value for seasonal variability as necessary.
- b – The average saturated thickness of the mixing zone is not necessarily equal to the full saturated thickness of the unconfined aquifer. In many shallow aquifers, particularly those comprised of stratified deposits, dissolved-phase groundwater contaminant plumes originating from the infiltration of vadose-zone leachate often remain located within the upper portions of the saturated zone (Domenico and Schwartz, 1998; Spitz and Moreno,

⁴ For example, the $C_{LEACHATE\ NO3}$ concentration prediction from NO3-LEACHATE-Scenario 3 will be carried forward for use in Scenario 3 of the GWNO3-FORECAST model.

1996). Ideally, the mixing zone thickness is determined from a site-specific characterization of the vertical distribution of nitrate within the aquifer, as well as the site hydrogeology. The b variable also may be estimated through calibration.

- dH and K_H – The hydraulic properties of the saturated mixing zone are best determined from site-specific hydrogeologic investigations (e.g., slug testing, aquifer testing, water level measurements).
- $C_{GW\ INFLOW\ NO_3}$ – This value is best determined from site-specific monitoring of conditions immediately upgradient of the site of interest. If a site measurement of upgradient nitrate-N concentration is unavailable, a default concentration for groundwater unaffected by human activities of 2 mg NO₃-N/L may be used (Tesoriero and Voss, 1997; Ryker and Frans, 2000; USGS, 1999; Madison and Brunett, 1985). The model user should, however, understand that many areas of Washington State have already been impacted by anthropogenic loading of nitrogen to groundwater. This suggests that current ambient background concentrations of nitrate-N at many sites in Washington may be elevated above what would occur naturally.

Users interested in determining the portion of the $C_{GW\ OUTFLOW\ NO_3}$ concentration that is specifically attributed to the leachate contribution can run a scenario with the $C_{GW\ INFLOW\ NO_3}$ term set to a value of zero (0). This removes from consideration any nitrate mass inputs from upgradient groundwater sources and highlights the effect of the site leachate on groundwater quality.

- AP_{SZ} – This value is also best determined from direct field evidence (see for example Carey and Harrison, 2014). If a site-specific value for this variable is unavailable, a default value of 0% is recommended for the initial model run (i.e., conservative transport). If the $C_{GW\ OUTFLOW\ NO_3}$ concentrations predicted by the GWNO3-FORECAST model are not in sufficiently close agreement with those measured in groundwater, the AP_{SZ} value may be determined through model calibration. Previous research has revealed that the denitrification capacity of aquifer systems may be limited and can be depleted over time, particularly in settings with high rates of surface irrigation and nitrogen application (Green and Bekins, 2010; Green et al., 2008).
- Field measurements of $C_{GW\ OUTFLOW\ NO_3}$ (for model calibration) – To calibrate the GWNO3-FORECAST model prediction to the nitrate concentration measured in groundwater, the user should account for the model assumptions when selecting the location(s) and screen interval position of the well(s) acting as the data source for this value.

Because the model assumes that the ambient groundwater and the leachate are fully mixed, the $C_{GW\ OUTFLOW\ NO_3}$ model predictions best represent an average steady-state condition, not necessarily the condition at any particular point. As a result, it is probably best to calibrate the model to a concentration that represents multiple well locations. Wells located in the downgradient portion of the site may better reflect the assumption of complete mixing than wells located near the upgradient model boundary. Data should be drawn from wells that are constructed with open intervals positioned at depths that are representative of the mixing zone thickness (b) selected for modeling.

Groundwater velocities and plume transport times may need to be considered when selecting field measurements of groundwater nitrate-N for the purpose of calibrating the model for a specific scenario. Although the model provides a steady-state concentration prediction, in the field there may be a time lag between the entry of the leachate into the aquifer and the arrival of the resulting leachate/groundwater mix at the selected observation well(s).

GWNO3-FORECAST Model Limitations

The GWNO3-FORECAST model greatly simplifies the process of a chemical solution entering and mixing with groundwater in an underlying aquifer. The model assumptions of uniformity and full mixing may not reflect real-world processes occurring in the subsurface. In reality, heterogeneity and anisotropy in the mixing zone aquifer material may result in incomplete mixing of the leachate with the inflowing groundwater (or non-uniform attenuation). In the field, this can lead to localized areas of the aquifer showing a significant impact from the leachate, while other areas may remain largely unaffected.

Similar to the NO3-LEACHATE model, GWNO3-FORECAST ignores the influence of time; the model simply assumes that the mixing of the leachate and ambient groundwater is complete by the end of the scenario period of interest. The model also ignores any delays in transport time of the vadose-zone leachate to the water table; that process is assumed to be complete by the beginning of the GWNO3-FORECAST scenario.

Users should remember that the GWNO3-FORECAST model predictions represent an average steady-state condition for the entire mixing zone volume. As a result, the user should take care to avoid unrealistic model scenarios or input values that significantly violate the model assumptions described above.

Model 3 - GWNO3-BACKCAST

GWNO3-BACKCAST Model Description

The four-step GWNO3-BACKCAST model is similar to Models 1 and 2, but the models are combined and equations modified to back-calculate the leachate concentration, nitrate mass load, and average shallow soil nitrate concentration values necessary to maintain a known or desired groundwater nitrate-N outflow concentration (Figure 4).

For the purpose of predicting the key model variables, the GWNO3-BACKCAST model differs from the NO3-LEACHATE model in two important ways: (1) the $NO3_{SUPP}$ term is not used in the model equations, and (2) soil nitrate concentration averages are back-calculated assuming that all nitrate mass derived directly from the vadose zone is distributed uniformly throughout the top 2 feet of the soil column.

In Step 1, a modified version of the mass balance equation (Equation 9, Model 2) is used to back-calculate the leachate concentration ($\bar{C}_{LEACHATE\ NO3}$) that will produce a given groundwater nitrate-N outflow concentration ($\bar{C}_{GW\ OUTFLOW\ NO3}$). The equation accounts for user-defined saturated zone attenuation processes (e.g., denitrification), aquifer conditions, and mixing.

Step 2 uses a modified version of Equation 8 from Model 1 to back-calculate the mass of leachable nitrate-N ($\overline{NO3}_{TOT\ LEACHABLE}$) required to produce the $\bar{C}_{LEACHATE\ NO3}$ value predicted by Step 1. User-defined leachate infiltration rate and vadose-zone attenuation effects are accounted for as necessary.

In Step 3, the nitrate-N mass contributed to the leachate by the recharge ($NO3_R$) is subtracted from the $\overline{NO3}_{TOT\ LEACHABLE}$ value, using a modified version of Equation 4. The result represents the nitrate mass that originates directly from within the vadose zone. Assuming that this mass is uniformly distributed within the top 2 feet of the soil column, the result is assigned the variable name: $\overline{NO3}_{LEACHABLE\ 0-2}$.

Finally, in Step 4, the model back-calculates the average 0-2 foot soil nitrate-N concentration ($\bar{C}_{SOIL\ NO3\ 0-2}$) from the $\overline{NO3}_{LEACHABLE\ 0-2}$ mass estimate (factoring in a user-defined average soil bulk density value for that portion of the soil column). This is the average soil nitrate-N concentration in the top 2 feet of the soil column that will maintain a given $\bar{C}_{GW\ OUTFLOW\ NO3}$ value, under the stated assumptions.

Model 3 can be run for ten independent model scenarios. Model predictions are automatically graphed by the spreadsheet file to allow visual evaluation of the results (Figure 5).

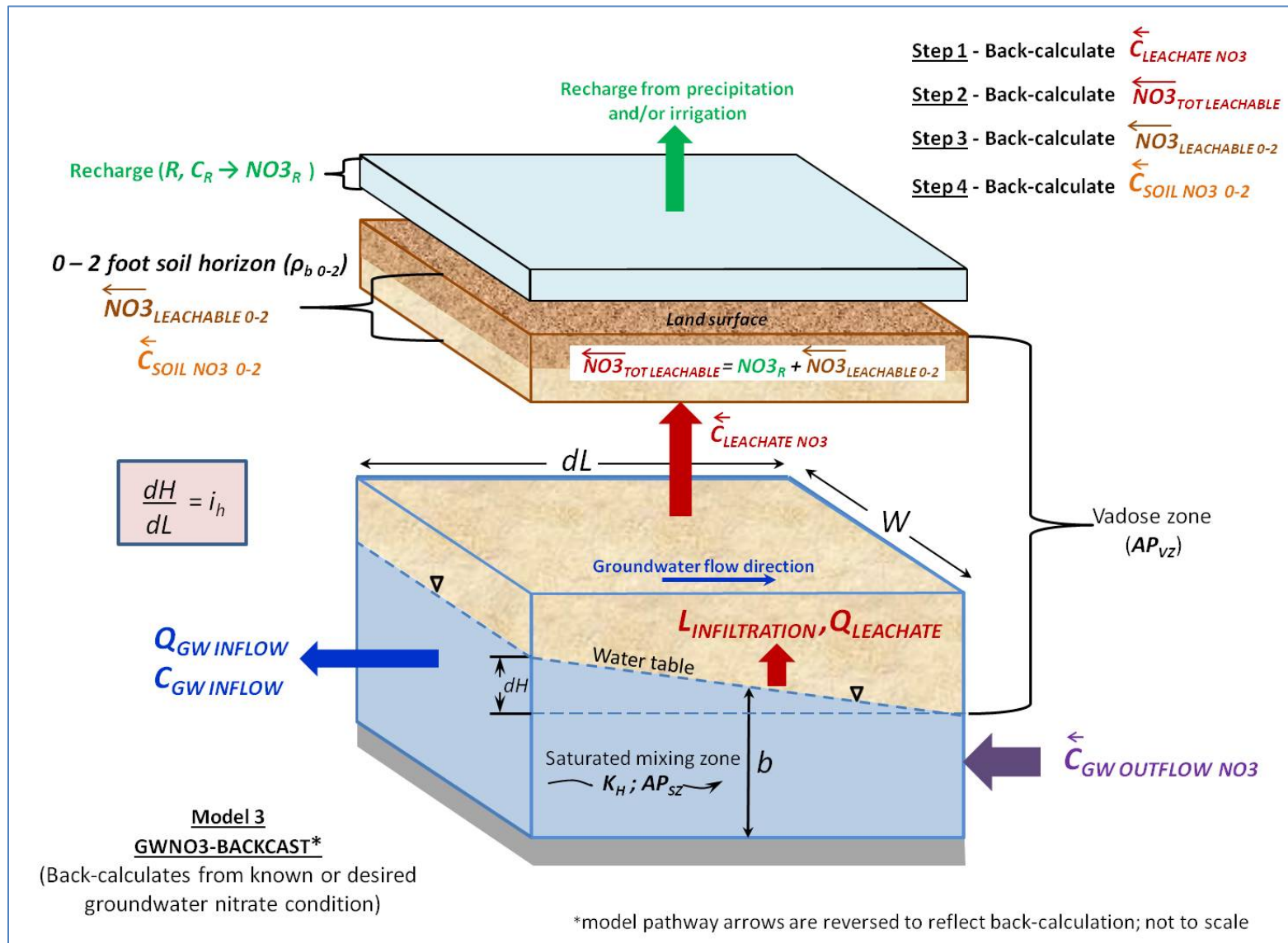


Figure 4. Conceptual Model Schematic – Model 3 (GWNO3-BACKCAST).

Refer to text for further explanation of figure symbols.

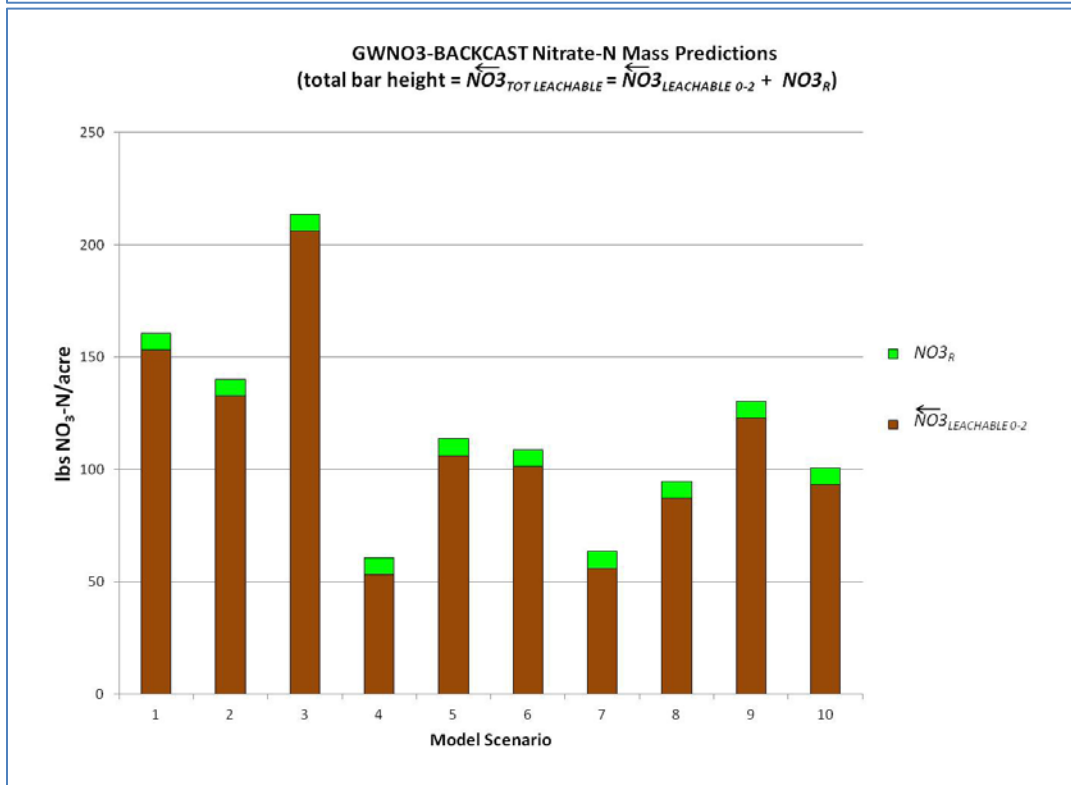
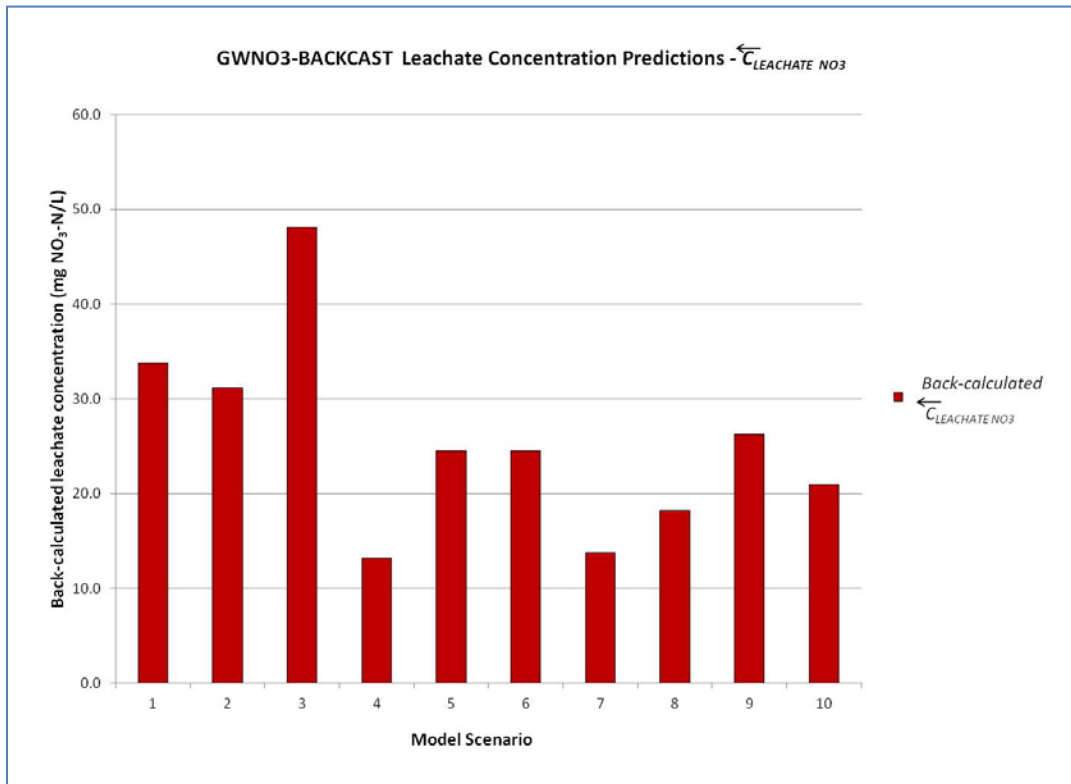


Figure 5. Example output graphs from the GWNO3-BACKCAST model spreadsheet.

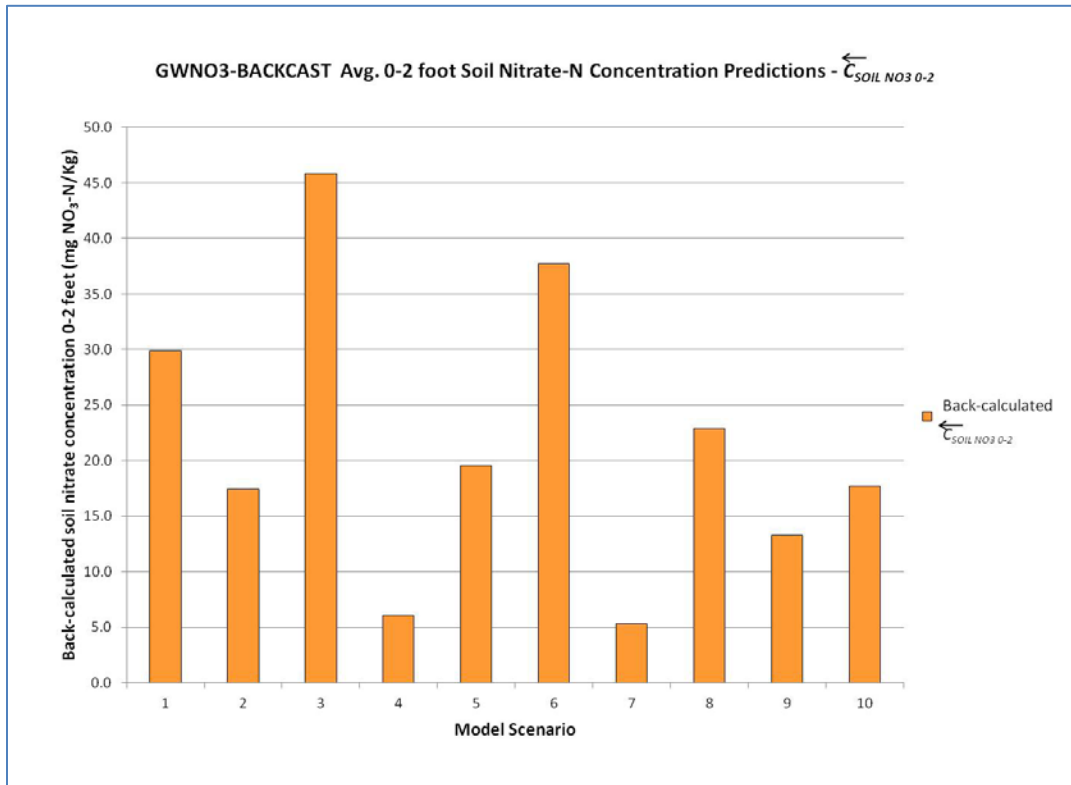


Figure 5 (cont.). Example output graphs from the GWNO3-BACKCAST model spreadsheet.

GWNO3-BACKCAST Model Equations

Step 1

To back-calculate the leachate concentration that will produce a given groundwater nitrate outflow concentration (under the stated assumptions), Equation 9 is modified to:

$$\bar{C}_{LEACHATE\ NO_3} = \frac{\bar{C}_{GW\ OUTFLOW\ NO_3}(Q_{LEACHATE} + Q_{GW\ INFLOW}) - [Q_{GW\ INFLOW} * C_{GW\ INFLOW\ NO_3} * (1 - \frac{AP_{SZ}}{100})]}{Q_{LEACHATE}(1 - \frac{AP_{SZ}}{100})} \quad (\text{Eq. 13})$$

where, for each model scenario:

$\bar{C}_{LEACHATE\ NO_3}$ = back-calculated concentration of nitrate-N in leachate that will produce a given $\bar{C}_{GW\ OUTFLOW\ NO_3}$ value (mg NO₃-N/L).

$\bar{C}_{GW\ OUTFLOW\ NO_3}$ = known or desired nitrate-N concentration in groundwater exiting the downgradient boundary of the saturated mixing zone at the end of the scenario period of interest (mg NO₃-N/L).

Step 2

The amount of leachable nitrate-N mass required to produce the predicted $\bar{C}_{LEACHATE\ NO_3}$ value from Step 1 is back-calculated by modifying Equation 8:

$$\overleftarrow{NO_3}_{TOT\ LEACHABLE} = \frac{2.719(R * \bar{C}_{LEACHATE\ NO_3})}{(1 - \frac{AP_{VZ}}{100})} \quad \text{Eq. 14}$$

where:

$\overleftarrow{NO_3}_{TOT\ LEACHABLE}$ = back-calculated leachable nitrate-N mass required to produce the $\bar{C}_{LEACHATE\ NO_3}$ value from Step 1 (lbs NO₃-N/acre).

Step 3

The nitrate-N mass contributed to the leachate directly from within the vadose zone can then be back-calculated using a modified version of Equation 4:

$$\overleftarrow{NO_3}_{LEACHABLE\ 0-2} = \overleftarrow{NO_3}_{TOT\ LEACHABLE} - NO_{3R} \quad \text{Eq. 15}$$

where:

$\overleftarrow{NO_3}_{LEACHABLE\ 0-2}$ = back-calculated nitrate-N mass contributed to the leachate from the vadose-zone soils (lbs NO₃-N/acre). *Assumes all nitrate mass directly originating from the vadose zone is uniformly distributed within the top 2 feet of the soil column.*

Step 4

Assuming that the Step 3 $NO_{3LEACHABLE\ 0-2}$ mass is uniformly distributed within the top two feet of the soil column:

$$\bar{C}_{SOIL\ NO_3\ 0-2} = \left(\frac{\overline{NO_{3LEACHABLE\ 0-2}}}{5.438\rho_{b\ 0-2}} \right) \quad \text{Eq. 16}$$

where:

$\bar{C}_{SOIL\ NO_3\ 0-2}$ = back-calculated average concentration of nitrate-N in the top 2 feet of the soil column required to produce a given $\bar{C}_{GW\ OUTFLOW\ NO_3}$ value (mg NO_3 -N/Kg DW).

$\rho_{b\ 0-2}$ = average soil bulk density for the 0-2 foot soil horizon (g/cm^3).

See Appendix A for the derivation of the conversion factors used in the above equations.

GWNO3-BACKCAST Model Assumptions

Most of the assumptions presented for Models 1 and 2 also apply to the GWNO3-BACKCAST model.

GWNO3-BACKCAST Model User-Defined Variables

The following variables can be defined by the user in the GWNO3-BACKCAST model:

- $\bar{C}_{GW\ OUTFLOW\ NO_3}$ – Model 3 can be used to develop predictions about the nitrate concentration and mass conditions necessary to maintain groundwater at or below a desired concentration (e.g., the state groundwater quality criterion of 10 mg NO_3 -N/L). Alternatively, it can be used to estimate the conditions that are required to explain a known groundwater concentration (e.g.: What nitrate concentration and mass loading conditions were necessary to produce the average groundwater nitrate concentration of 36 mg NO_3 -N/L I observed near the downgradient boundary of my study field?).
- $C_{GW\ INFLOW\ NO_3}$ – see notes for this variable in the Model 2 section (“GWNO3-FORECAST User-Defined Variables”).
- AP_{SZ} – see notes for this variable in the Model 2 section.
- dL and W – see notes for these variables in the Model 2 section.
- $L_{INFILTRATION}$ – see notes for this variable in the Model 2 section.
- b (used in Eq. 11 to compute $Q_{GW\ INFLOW}$) – To determine the amount of nitrate-N loading that will result in a given concentration of nitrate in groundwater *at the water table*, the user should set this value to zero (0). Doing so also sets $Q_{GW\ INFLOW}$ to zero, removing from consideration mixing and dilution within the saturated zone, and resulting in the assumption that $\bar{C}_{LEACHATE\ NO_3} = \bar{C}_{GW\ OUTFLOW\ NO_3}$ (assuming AP_{VZ} and AP_{SZ} are set to 0%).

To determine the loading required to produce a given $\bar{C}_{GW\ OUTFLOW\ NO_3}$ value after mixing within the aquifer has occurred, the user should set the value of b to reflect the assumed vertical extent of mixing. See additional notes for this variable in the Model 2 section.

- K_H and dH (used in Eqs. 11 and 12 to compute $Q_{GW\ INFLOW}$) – These values are best determined from site-specific investigations.
- R – see notes for this variable in the Model 1 section (“NO₃-LEACHATE Model User-Defined Variables”).
- AP_{VZ} – see notes for this variable in the Model 1 section.
- $C_{R\ NO_3}$ – see notes for this variable in the Model 1 section.
- $\rho_{b\ 0-2}$ – see notes for estimation of soil bulk density in the Model 1 section and in Appendix B. This value should represent the average bulk density for the top 2 feet of the soil column.

GWNO3-BACKCAST Model Limitations

All of the limitations described for Models 1 and 2 also apply to GWNO3-BACKCAST. The assumption that the leachable nitrate mass directly derived from the vadose zone is entirely concentrated within the top 2 feet of the soil column ignores the possibility that some of that mass could actually originate from below 2 feet. The assumption that the $NO_{3\ LEACHABLE\ 0-2}$ nitrate mass is *uniformly* distributed within the 0-2 foot soil horizon results in a prediction of the *average* soil nitrate concentration that would produce the given $\bar{C}_{GW\ OUTFLOW\ NO_3}$ value. In the field, soil nitrate is often not uniformly distributed with depth.

Spreadsheet Models

The three models described above have been incorporated into an interactive Excel 2007[®] file. Instructions for using the models are embedded in the spreadsheet file. Model predictions are automatically graphed and, if appropriate, can be compared to field-collected data for calibration purposes.

It is recommended that users thoroughly review the information in this publication, with a particular eye toward understanding the model assumptions and limitations, before applying the models to site-specific loading analyses.

Conclusions and Recommendations

- The three models described in this report represent a significant simplification of the real world. The different assumptions used by the model can lead to either under-predictions or over-predictions of actual (i.e., measured) concentration and mass values, depending on how well those assumptions align with existing conditions *in situ*. These models are therefore best used for rapid, low-cost screening analyses, range-finding exercises, and scenario comparison (e.g.: What will happen if we reduce the nitrate-N concentration of the irrigation water we apply? Is site A more vulnerable to groundwater contamination than site B? What sort of nitrate mass loading is required to explain the existing groundwater nitrate condition we see at our site?). The more the user can rely on site-specific field measurements to inform the input values, and the closer the tested scenarios adhere to the model assumptions, the less uncertainty there will be in the model predictions.
- Calibration of the GWNO3-FORECAST predictions to nitrate concentrations measured in groundwater can strengthen user confidence in those predictions and may help reveal processes that are perhaps otherwise difficult to quantify in the field. For example, some users may observe insufficient agreement between model predictions and field measurements unless they increase the input values for supplemental nitrate mass in the vadose zone. This suggests the possibility that previously unrecognized mineralization of organic nitrogen may be occurring at their site, or that other sources of nitrate have not been accounted for. This approach may also reveal denitrification that had not been previously detected. Users are reminded that model solutions are not necessarily unique (i.e., there may be multiple combinations of input variable values that can produce the same model prediction).
- The models also can be a useful tool for sensitivity analyses, to determine which input parameters have the greatest or least influence on the prediction results. Sensitivity analyses can be a cost-effective way to identify priorities for more in-depth field investigation. For example, if the model predictions are found to be highly sensitive to the amount of recharge, additional field measurements and quantitative analysis of recharge may be justified to increase confidence in the model predictions. Varying a single parameter over multiple scenarios, while fixing all other input parameters at appropriate constant values, is a simple way to conduct a sensitivity analysis. For advanced users interested in using automated tools to run multi-parameter sensitivity and uncertainty analyses, we recommend tools such as the Department of Ecology's freeware YASAIw add-on for Excel (see: www.ecy.wa.gov/programs/eap/models.html), or proprietary software such as Oracle's Crystal Ball.
- The models are designed to predict spatially averaged, steady-state conditions; they are not intended to predict nitrate loading or concentrations at any particular point in the subsurface. Several simplifying assumptions, such as complete mixing, limit the usefulness of the models for very short periods of time; the models are best suited for longer-term analyses.
- Because the models described in this report significantly simplify the processes controlling the fate and transport of nitrate in both the vadose zone and the saturated zone, the model predictions should not be used as a replacement for direct monitoring of groundwater conditions.

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Appendices

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Appendix A. Derivation and Units of Conversion Factors

A.1 Soil concentration-to-mass unit conversion

To convert a 1-foot thick soil sample nitrate-N concentration in units of mg/Kg to a nitrate-N mass value in units of lbs/acre, first:

$$\frac{1 \text{ kg}}{1000000 \text{ mg}} * \frac{1000 \text{ mg}}{1 \text{ g}} * \frac{2.205 * 10^{-6} \text{ lbs}}{1 \text{ mg}} * \frac{1.233 * 10^9 \text{ cm}^3}{1 \text{ acre ft}} = 2.719 \frac{\text{kg lbs cm}^3}{\text{g mg acre ft}} \quad \text{Eq. A.1}$$

Combining the units above with the units for soil bulk density and soil volume yields:

$$\frac{\text{kg lbs cm}^3}{\text{g mg acre ft}} * \frac{\text{g}}{\text{cm}^3} * \frac{1 \text{ acre ft}}{\text{acre}} = \frac{\text{kg lbs}}{\text{mg acre}} \quad \text{Eq. A.2}$$

Then, multiplying the Eq. A.2 units by the given soil nitrate-N concentration units:

$$\frac{\text{kg lbs}}{\text{mg acre}} * \frac{\text{mg}}{\text{kg}} = \frac{\text{lbs}}{\text{acre}} \quad \text{Eq. A.3}$$

In the GWNO3-BACKCAST model, the conversion factor of 2.719 is multiplied by 2 (2.719*2=5.438) to help convert a nitrate-N soil mass back to an average 0-2 foot soil nitrate-N concentration.

A.2 Dissolved phase concentration-to-mass unit conversion

To convert a dissolved phase nitrate concentration in recharge, in units of mg/L, to a mass value in units of lbs/acre, first:

$$\frac{2.205 * 10^{-6} \text{ lbs}}{1 \text{ mg}} * \frac{1.233 * 10^6 \text{ L}}{1 \text{ acre ft}} = 2.719 \frac{\text{lbs L}}{\text{mg acre ft}} \quad \text{Eq. A.4}$$

Combining the conversion factor units with the units for recharge volume and recharge concentration yields:

$$\frac{\text{lbs L}}{\text{mg acre ft}} * \frac{\text{acre ft}}{\text{acre}} * \frac{\text{mg}}{\text{L}} = \frac{\text{lbs}}{\text{acre}} \quad \text{Eq. A.5}$$

A.3 Volume-to-volume unit conversion

$$\frac{28.32 \text{ L}}{\text{ft}^3} * \frac{\text{ft}^3}{\text{day}} = \frac{\text{L}}{\text{day}} \quad \text{Eq. A.6}$$

Appendix B. Soil Bulk Density

This appendix presents analyses of bulk density value ranges for cropland soils in eastern and western Washington. The analyses were conducted and reported by Steve Campbell, Soil Scientist with the U.S. Dept. of Agriculture, Natural Resources Conservation Service (NRCS), West National Technology Support Center. Data for the analyses were drawn from the NRCS Soil Survey Geographic Database (SSURGO). Bulk density value ranges are presented for the 0-30 cm (~0-12") and the 30-60cm (~12-24") depth-intervals.

Spreadsheets of the raw SSURGO data compiled for the analysis (by soil map unit) are available as supplemental files to this report (to support site-specific bulk density determinations).

Soil Bulk Densities in Eastern Washington Soils used for Cropland - June 2014

SSURGO soil survey bulk density data for the 0-12 inch (0-30 cm) and 12-24 inch (30-60 cm) depths were evaluated for soils used for cropland in Major Land Resource Areas 7, 8, and 9 in Eastern Washington. In general, sandy soils have the highest bulk density, loamy soils are intermediate, and clayey soils have the lowest bulk density (www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/nrcs142p2_053256.pdf). The table below from the Soil Survey Manual, Chapter 3, contains groupings of soil texture classes (www.nrcs.usda.gov/wps/portal/nrcs/detail/soils/ref/?cid=nrcs142p2_054253).

<i>General Terms^a</i>	<i>Texture Classes</i>
Sandy soil materials:	
Coarse	Sands (coarse sand, sand, fine sand, very fine sand) Loamy sands (loamy coarse sand, loamy sand, loamy fine sand, loamy very fine sand)
Loamy soil materials:	
Moderately coarse	Coarse sandy loam, sandy loam, fine sandy loam
Medium	Very fine sandy loam, loam, silt loam, silt
Moderately fine	Clay loam, sandy clay loam, silty clay loam
Clayey soils:	
Fine	Sandy clay, silty clay, clay

Range of Eastern Washington Soil Bulk Densities for Cropland Soils (grams per cubic centimeter).

Texture Class Group	Count	Low bulk density	Average bulk density	High bulk density
Coarse, 0-12 in.	154	1.30	1.50	1.60
Coarse, 12-24 in.	188	1.35	1.55	1.65
Moderately coarse, 0-12 in.	547	1.20	1.30	1.50
Moderately coarse, 12-24 in.	371	1.25	1.35	1.55
Medium, 0-12 in.	1761	1.15	1.25	1.45
Medium, 12-24 in.	1652	1.20	1.30	1.50
Moderately fine, 0-12 in.	79	1.15	1.25	1.45
Moderately fine, 12-24 in.	258	1.20	1.30	1.50
Fine, 0-12 in.	14	1.10	1.20	1.35
Fine, 12-24 in.	86	1.15	1.30	1.50
Organic, 0-12 in.	1	0.20	0.20	0.25
Organic, 12-24 in.	1	0.20	0.20	0.25

Contact for questions:

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Soil Bulk Densities in Western Washington Soils used for Cropland - June 2014

SSURGO soil survey bulk density data for the 0-12 inch (0-30 cm) and 12-24 inch (30-60 cm) depths were evaluated for soils used for cropland in Major Land Resource Area 2 in Western Washington. In general, sandy soils have the highest bulk density, loamy soils are intermediate, and clayey soils have the lowest bulk density (www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/nrcs142p2_053256.pdf). The table below from the Soil Survey Manual, Chapter 3, contains groupings of soil texture classes (www.nrcs.usda.gov/wps/portal/nrcs/detail/soils/ref/?cid=nrcs142p2_054253).

<i>General Terms^a</i>	<i>Texture Classes</i>
Sandy soil materials:	
Coarse	Sands (coarse sand, sand, fine sand, very fine sand) Loamy sands (loamy coarse sand, loamy sand, loamy fine sand, loamy very fine sand)
Loamy soil materials:	
Moderately coarse	Coarse sandy loam, sandy loam, fine sandy loam
Medium	Very fine sandy loam, loam, silt loam, silt
Moderately fine	Clay loam, sandy clay loam, silty clay loam
Clayey soils:	
Fine	Sandy clay, silty clay, clay

Range of Western Washington Soil Bulk Densities for Cropland Soils (grams per cubic centimeter).

Texture Class Group	Count	Low bulk density	Average bulk density	High bulk density
Coarse, 0-12 in.	125	1.00	1.40	1.65
Coarse, 12-24 in.	236	1.05	1.45	1.65
Moderately coarse, 0-12 in.	342	0.75	1.15	1.55
Moderately coarse, 12-24 in.	312	0.75	1.20	1.85
Medium, 0-12 in.	597	0.70	1.10	1.50
Medium, 12-24 in.	395	0.75	1.15	1.55
Moderately fine, 0-12 in.	98	0.75	1.20	1.40
Moderately fine, 12-24 in.	163	0.90	1.25	1.45
Fine, 0-12 in.	8	0.95	1.20	1.45
Fine, 12-24 in.	68	1.20	1.30	1.50
Organic, 0-12 in.	69	0.20	0.25	0.50
Organic, 12-24 in.	65	0.20	0.25	0.5

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Appendix C. Estimated Background Concentrations of Dissolved Nitrate-N Concentrations in Washington State Precipitation

To provide the basis for a default assumption for the background or initial concentration of nitrate (nitrate-N or NO₃-N) in rainfall-derived recharge, precipitation-weighted annual mean concentration data from the National Atmospheric Deposition Program (NAPD) website (<http://nadp.sws.uiuc.edu/>) were compiled from seven National Trends Network (NTN) stations (see Table A-1). Data from five of these stations were used to calculate a composite average value for western Washington; data from the other two stations were used to calculate a composite average value for eastern Washington.

Table A-1. Precipitation-weighted annual mean nitrate-N concentration data from selected Washington State monitoring stations (source: NAPD).

NADP NTN Station ID	County, State	Latitude	Longitude	Data Period	Average NO ₃ -N Concentration (mg/L)	95% Confidence Interval (mg/L)
Western Washington						
WA14	Jefferson, WA	47.8597	-123.933	2002-2012	0.022	±0.002
WA19	Skagit, WA	48.5403	-121.446	2002-2012	0.059	±0.004
WA21	Pierce, WA	46.8353	-122.287	2002-2012	0.065	±0.006
WA98	Skamania, WA	45.5694	-122.21	2002-2012	0.064	±0.008
WA99	Pierce, WA	46.7582	-122.124	2002-2012	0.042	±0.004
Composite average NO ₃ -N concentration (mg/L)* : 0.05						
Eastern Washington						
WA24	Whitman, WA	46.7606	-117.185	2003-2012	0.086	±0.007
ID02	Bonner, ID	48.3518	-116.84	2003-2012	0.088	±0.009
Composite average NO ₃ -N concentration (mg/L)*: 0.09						

*NTN data are reported as NO₃ in mg/L. These values were converted to NO₃-N using a conversion factor of 0.2259.

Appendix D. Units of Measure and Conversion Factors

Units of Measure

acre-ft	acre-foot
L	liters
L/day	liters per day
mg NO ₃ -N/Kg	milligrams nitrate as nitrogen per kilogram = parts per million
ft	feet
lbs NO ₃ -N/acre	pounds nitrate as nitrogen per acre
lbs N/acre	pounds nitrogen per acre
mg NO ₃ -N/L	milligrams nitrate as nitrogen/liter
g/cm ³	grams per cubic centimeter
ml/g	milliliters per gram

Appendix E. Supplemental Microsoft Excel 2007 Files

Three Microsoft Office Excel 2007[®] worksheet files are included with this report:

- ***NO3_MB_loading_models_V1.0.xlsx***
This worksheet file contains the three spreadsheet models described in this report (NO3-LEACHATE, GWNO3-FORECAST, and GWNO3-BACKCAST).
- ***USDA_Campbell_W_WA_soil_BD_data.xlsx***
This worksheet file contains soil bulk density data for crop soils in western Washington, drawn from the NRCS SSURGO database (Campbell, 2014).
- ***USDA_Campbell_E_WA_soil_BD_data.xlsx***
This worksheet file contains soil bulk density data for crop soils in eastern Washington, drawn from the NRCS SSURGO database (Campbell, 2014).

These Excel files are available only on the Internet, linked to this report at <https://fortress.wa.gov/ecy/publications/SummaryPages/1403018.html>