

Instructions for Spreadsheet GPL

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Introduction

The Spreadsheet GPL is an Excel spreadsheet that duplicates the calculations of the Fortran based 1996 Groundwater Protection Leaching (GPL) model. Its primary purpose is to accurately reproduce the GPL model in a spreadsheet format that allows Users to run the model, view calculations, and print out results.

The GPL model is described in detail in the 1996 publication *A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality*. Spreadsheet users should be familiar with the leaching guidance before using the spreadsheet GPL.

GPL Revisions

The Spreadsheet GPL calculations are different than the 1996 GPL model in three significant ways. Two of the changes directly affect the calculations. The third allows calculation of GPLs for additional chemicals. The three changes are explained below.

1) The maximum GPL may now be capped based upon chemical saturation considerations. The spreadsheet GPL calculates a total soil contaminant concentration assuming a chemical is present in the liquid phase at the solubility limit. The saturation value is then compared to the GPL calculation and a warning is given if the GPL exceeds the saturation level. The change was made because of the equilibrium partitioning equations and concerns regarding the movement of free phase contamination.

The GPL calculations assume that the equilibrium concentration in all soil phases is directly proportional. However, at the water solubility limit, vapor and liquid concentrations are at the maximum. Soil gas and liquid phase concentrations will not increase above the threshold no matter how much more contaminant is added to the soil. Ignoring the solubility threshold causes the GPL to calculate unrealistically high vapor and liquid phase concentrations.

Free phase contaminants may be present if the measured soil total contaminant concentration exceeds the saturation value. Laboratory studies of hydrocarbons indicate that movement of free phase between soil pores may occur when between 3- 8% of the pore volume is occupied by the free-phase. However, free phase movement in the vadose zone is a complex phenomena which can be affected by even small changes in soil texture and moisture content. If the measured soil concentration exceeds the saturation value, the site data should be reviewed to determine whether the GPL is a suitable model for estimating groundwater impacts.

Under all circumstances the residual concentration in the soil cannot 1) cause or threaten contamination of groundwater to exceed an Aquifer Water Quality Standard (AWQS), 2) cause or threaten to cause a violation of a surface water quality standard, and 3) exhibit the ignitability, corrosivity or reactivity characteristic of hazardous waste.

2) The chemical properties for volatility (K_h - Henry's constant) and soil distribution coefficient (K_{oc}) have been revised. Both properties have been updated for the chemicals of concern and are now consistent with the chemical properties used to calculate Soil Remediation Levels (SRLs). A worksheet titled **Minimum GPLs** is included in the Spreadsheet GPL that compares the 1996 and the new minimum GPLs.

3) Minimum GPLs can now be calculated for additional chemicals. The calculation requires a water quality standard but many of the additional chemicals do not have an Aquifer Water Quality Standard (AWQS). In these cases, a risk-based water standard is used in lieu of the AWQS. However, risk-based groundwater concentrations may not have the regulatory authority of AWQS. The Lookup Table work-sheet details all of the chemicals included in the data base.

GPL Additions

The spreadsheet includes additional options such as:

- 1) A worksheet titled **Soil Phase Partitioning** that calculates soil phase equilibrium concentrations.
- 2) A worksheet titled **IntercalcsJury2** that estimates soil concentration changes with depth at a specific time.
- 3) A worksheet titled **IntercalcsJury1** that estimates groundwater and vadose zone impacts for any initial soil concentration.

Operating Instructions

The Spreadsheet GPL is an Excel spreadsheet constructed to duplicate the Fortran based 1996 GPL model. The input requirements for both models are identical. Data is added to the spreadsheet through the Input worksheet and minimum GPL values are displayed at the bottom of the worksheet. Drop down boxes are provided in the Input worksheet screen for entering soil and chemical properties. The information in the drop down boxes is shown in the Look Up Table work sheet.

The spreadsheet version of the GPL makes it easy to modify the model inputs. However, model inputs should not be changed from the default values unless justified by site-specific information. The chemical properties used in the drop down boxes were adopted from the Soil Remediation Levels (SRLs). Other default values are listed on the Input work sheet and described in the 1996 publication *A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality*.

Visual Basic Applications (VBA) are included to solicit user preferences for GPL default values, half life, and time step calculations. Automated and manual time step options are available. The output graphs must be carefully reviewed to ensure peak vadose zone concentrations are captured in the calculations.

Output from the spreadsheet calculations is graphed and presented in the Output work sheets. The worksheets are protected but all of the formulas are visible. A work sheet titled Intercalcs Jury2 calculates the concentration of soil contamination across the vadose zone at a user specified time. A worksheet allows users to calculate equilibrium soil and soil gas concentrations.

Calculating a GPL

- 1) Open the Spreadsheet GPL and select Input worksheet. It may be necessary to load the Analysis Tool Pack by opening the spreadsheet windows Tools, Add-Ins, and checking the Analysis Toolpack box.

Two columns affect the calculations. The first column "Calculation values" shows the inputs used in the calculations. A second column "Data Enter" is used to enter site specific information and facilitate data entry. Only the data in the "Calculation values" column is used in the calculations

- 2) Select a chemical from the approximately 70 chemicals listed in the row 6 drop down list. Values for Koc, Kh, solubility, and a water quality standard for that specific chemical are automatically placed in the appropriate row in the blue column. A GPL for a specific chemical should be calculated only with that chemical's properties. The parameters for each chemical are listed in the Lookup Table work sheet.

For chemicals not listed in the drop down list, select 'Enter chemical properties' and enter values for Koc, Kh, and a water quality standard into the appropriate cells in the blue column.

- 3) Enter an initial total soil contaminant concentration in ug/kg into row 7 of the blue column. The soil concentration does not affect the GPL calculation, unless zero is entered, because the model calculates the total soil concentration that will just produce a groundwater concentration equal to the specified water quality

standard. However, the vadose zone and groundwater impacts increase with increasing concentrations which can be seen by viewing the output graphs.

- 4) Enter an appropriate biodegradation half life in the blue column of rows 11 and 12. The biodegradation rate may be different in the vadose zone and groundwater but typically they are the same.

For BTEX compounds, the assumed half life is 1000 days. Chlorinated compounds are assumed to be relatively non biodegradable and a half life of 100,000 days is assumed. See the Leaching Guidance for a discussion of biodegradation rates. Default values can be selected from the "Run GPL" button.

- 5) Select a soil type from the drop down list in row 13 of the blue column. Values for moisture content, bulk density, and porosity for that specific soil type are automatically placed into the appropriate cells in the blue column. Other soil properties may be appropriate based upon site specific information. The soil properties for each soil type are listed in the Lookup Table.

For soil types not listed in the drop down box, select "New soil type" and enter the required soil properties in the appropriate cell of the blue column. The values are automatically copied into the calculation column. The soil properties shown in the Lookup Table are approximate. Deviations from the GPL defaults must be based upon a site specific geotechnical analysis of the soil.

- 6) Enter the remaining model inputs. Default values are listed to the right of the variable. Most GPL defaults can be quickly entered by selecting the "Insert GPL Defaults" check box that is within the "Run GPL" button. The default button automatically makes the depth to groundwater equal to the depth of incorporation resulting in a minimum GPL. Other GPL values can be calculated by modifying the defaults. See the 1996 publication *A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality* Leaching Guidance for a discussion of default values.

- 7) Determine a time step for the model. The time step is the time interval in days at which concentrations are calculated. Peak vadose zone concentrations are used in the GPL calculations and can vary significantly depending primarily upon the difference between the depth of incorporation and the depth to groundwater, chemical volatility, infiltration rates, and groundwater velocity.

Two options are available for a time step. The "Automatic time step" check box calculates an initial time step that usually captures the peak concentration. The liquid phase concentration over time graph in the Output Jury1 work sheet must be viewed to ensure the peak value has been calculated at an appropriate

resolution. The calculated value is automatically copied into the appropriate cell in row 24.

If the “Automatic time step” button does not result in a suitable time step, the “manual time step” button should be selected. A time step in days is entered. Again, the liquid phase concentration over time graph in the Output Jury1 work sheet must be viewed to ensure the peak value has been calculated at an appropriate resolution.

- 8) View the results. Row 45 of the Input work sheet displays the GPL and information about the calculation. If the GPL exceeds the solubility threshold, a note appears. Similarly, it is noted whether the GPL is calculated based upon a risk-based or Aquifer Water Quality Standard.

Jury2 Solution

The Jury2 solution estimates soil contaminant concentrations across the vadose zone at a specific time. Site specific concentration data can be compared with the theoretical contaminant distribution predicted by the Jury2 model to assist in understanding contaminant movement.

As an example, Figure 1 illustrates the change in TCE soil gas concentration over time with GPL defaults and an initial depth of incorporation of 10 meters. The graph illustrates the spreading of contamination over time, which at low water infiltration rates is primarily due to diffusive gas transport of TCE. Other observations include diminishing peak concentrations and increasing concentrations with depth due to contaminant losses through the surface.

The data requirements for the Jury2 solution are the same as the Jury1 solution. However, a specific time and vadose zone depth must be entered in rows 27 and 28, respectively. Also, the “Run GPL” button is not needed for the Jury2 solution. The calculation is performed automatically with the data shown in the “Calculation values” column.

Soil Phase Partitioning

The Soil phase partitioning worksheet is used to calculate equilibrium contaminant concentrations in the soil gas, soil liquid and total contaminant phases. Drop down boxes are provided for chemical and soil type that are identical with the Input worksheet. A VBA procedure is included to solicit User Input. Saturation concentrations are calculated and a notification is given if the total contaminant concentration exceeds solubility limits.

To calculate equilibrium concentration, chemical and soil types are selected from the drop down boxes. For an unlisted chemical or soil type, the “Enter chemical property” or

“new soil type” is selected and the properties entered in the appropriate cells in the Data Enter column.

The last step in the procedure is to click on the “Calculate Soil Phase Calculations” button, check the appropriate box and then enter the numeric data for the concentration phase that correspond to the check box. The concentrations in the other phases are then listed on the bottom of the page. It is necessary to click on the button anytime a spreadsheet value is changed in order to calculate a new equilibrium concentration distribution.

Work sheet descriptions

Details regarding the specific worksheets are listed below.

1) Instructions:

Work sheet 1 includes a brief discussion regarding each of the work sheets. Users should be familiar with *A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality*.

2) Diagram:

This work sheet duplicates Figure 1 in Appendix B of the document “*A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality* “. The labeling of the variables is consistent with the Input sheet.

3) Minimum GPLs:

This table shows the minimum GPLs with revised chemical properties and GPL defaults in comparison with earlier GPLs. Saturation concentrations are also included.

4) Lookup Table:

This table shows chemical property information for 70 chemicals and soil property information for various soil types. The chemical and soil properties from the Input sheet are linked to this table. A distinction is made in the table for chemicals with Aquifer Water Quality Standards (AWQS) versus those with only risk- based values. The Input worksheet includes a statement regarding which standard is used in the GPL calculation.

The soil properties shown in the Lookup Table are approximate. Deviations from the GPL defaults must be based upon a site specific geotechnical analysis of the soil.

5) Inputs:

This work sheet is used to enter data and view the results of the GPL calculations. Two columns affect the calculations. The first column “Calculation values” shows the inputs used in the calculations. A second column “Data Enter” is used to enter site specific information and facilitate data entry. Only the data in the “Calculation values” column is used in the calculations.

Specific information regarding the data is available in the 1996 publication *A Screening Method to Determine Soil Concentrations Protective of Groundwater Quality Leaching Guidance*. One difference between the spreadsheet and the Fortan model is the spreadsheet allows the initial soil contaminant concentration to be manipulated.

6) IntercalsJury1:

This worksheet displays the calculations for the Jury model upon which the GPL is based. No data entry is required. The input requirements are copied from the Input worksheet. The results from this work sheet are graphed in the OutputJury1 work sheet.

7) OutputJury1:

This work sheet graphs the data from the IntercalsJury1 work sheet of concentration versus time for three vadose zone soil phases: air, water, and solid. Also included are the ratio of concentration/ initial concentration versus time and total soil contamination versus time. Total soil contamination is the sum of contamination from all 3 phase.

8) GPL:

This work sheet calculates the GPL given the data from the Input worksheet. No information needs to be entered. It is included to allow users to view the calculations. The GPL result from the calculation is also displayed on the Input page.

9) IntercalsJury2:

This work sheet displays the calculations from the Jury2 model. The Jury2 model predicts soil concentrations across the vadose zone at a specific time. No data entry is required. The input requirements are copied from the Input work sheet. The results from the work sheet are graphed in the OutputJury2 work sheet.

10) OutputJury2:

This work sheet graphs the data from the IntercalsJury2 work sheet of concentration versus time for three vadose zone soil phases: air, water, and solid. Also included are the ratio of concentration/ initial concentration versus time and total soil contamination versus time. Total soil contamination is the sum of contamination from all 3 phases.

11) Soil Phase Partitioning

This worksheet calculates the equilibrium air, liquid, and total soil contaminant concentrations.

Deviation from Model Inputs

The responsibility for demonstrating that the model results are protective of groundwater quality lies with the party conducting the analysis. The default model inputs were selected to be reasonable and without bias regarding effects on resulting screening levels. Departures from the model defaults should be done carefully. Documentation detailing

the rationale for deviations from the model defaults is required. ADEQ programs should be consulted to discuss any model changes that involve regulatory issues.

Troubleshooting

1) Spreadsheet won't run.

Problems opening the spreadsheet are usually caused by certain mathematical functions not being loaded. The error function and the complimentary error functions are needed to run the model. To correct the problem load the Analysis Tool Pack by opening the spreadsheet windows Tools, Add-Ins, and checking the Analysis Toolpack box.

2) The Input GPL worksheet states #Div/0!.

a) The peak liquid phase vadose zone concentration is equal to zero. Try a different time step and view the OutputJury1 graph for liquid phase concentrations. Continue to change the time step until a peak concentration is displayed.

b) The initial soil contamination input is zero. Change to a non-zero number and rerun the spreadsheet.

3) Can not duplicate the minimum GPL values.

Review the model input parameters for correct entry. In particular, an incorrect half life is often used.

4) Graphs from the Output worksheets indicate concentrations are still increasing.

Modify the time step until the peak concentration is displayed. More accurate results are obtained with smaller time steps.

Figure 1: Soil gas concentration versus time, Initial Depth of incorporation = 10 meters

