

JAVA Program for Calculation of Attenuation Factor of Pesticides*

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Abstract

The Attenuation Factor (AF) value is an index of the relative likelihood of ground water contamination computed on the basis of the percent of applied chemical leaching beyond the surface soil layers. The Attenuation Factor Calculator (AFC) Program is used to automate the process of calculating the Attenuation Factor (AF) of pesticides as they leach through the soil layers/horizons. The program is written in JAVA and provides a user friendly interface to a)load the pesticides' database; b)load maps; c)calculate the AF at any desired depth in the soil profile, OR at the end of any layer OR at the depth to ground water for the selected pesticide; d)save output maps; e)filter the values in a map. The AF calculation requires parameters such as Bulk Density (BD), Organic Content (OC), Depth below the ground surface (D) and pesticide Sorption (K_{oc}) and Half Life ($t_{1/2}$) values which can be loaded in the program using simple text files. These text files can be brought in the desired format using a Toolbox provided with the program. The program has been tested on various counties in Arkansas and Florida states and the AF maps generated by AFC are verified by calculating the AF manually at some sample points in the map.

Keywords: Attenuation Factor; Pesticides; JAVA; Leaching

1. Introduction

Groundwater is a major source of drinking water for animals and human beings. Once the groundwater is contaminated, it is an extremely costly operation to remove the contaminant. Any chemicals that are easily soluble and penetrate the soil are the prime candidates of groundwater pollutants. Each year, 3.5 million to 21 million pounds of pesticides reach ground or surface water before degradation [1].

* Code is available at http://www.stpt.usf.edu/bdixon/gal/projects_final.html

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Thus, it is necessary to study the various environmental processes that influence pesticide dynamics in soils to predict the potential of a particular pesticide to reach into the groundwater [1]. The potential of an organic compound, such as a pesticide, depends on its mobility. Mobility assessment of pesticides involves both indirect and direct approaches. The indirect approach involves the measurement of an indicator parameter, which is used as an index for the relative ranking of mobility of organic chemicals. Several parameters, including sorption coefficient, retardation factor, molecular connectivity, and parachor have been used by various investigators [1, 2]. Direct assessment of

mobility is accomplished by using complex mathematical models that describe the transport of the organic compounds in soil systems. The contamination potential of a pesticide may be evaluated by the likelihood of a chemical to pass through the biologically active surface soil horizons (usually top 1 m). The Attenuation Factor (AF) value is an index of the relative likelihood of ground water contamination computed on the basis of the percent of applied chemical leaching beyond the surface soil layers [3]. AF values range from 0 to 1; a value of 0 implies that none of the applied chemical is likely to contaminate the well; whereas a value of 1 indicates all of the chemical may leach into a well. We have implemented a JAVA program called Attenuation Factor Calculator (AFC) for calculating the AF. The AFC is unique because it can be used to calculate the AF at any layer of the soil profile or at the depth to ground water or at any depth in the soil profile.

The paper is organized as follows. The following section gives the mathematical background of AF calculation process, followed by a section explaining the algorithm and the usage of AFC. The examples section shows the output of the program for a sample county. The future work section explains possible amendments in the existing program.

2. Mathematical Background

The AF computations require soil and climatic data in addition to pesticide chemical properties. Equation (1) is used to calculate the AF.

$$AF = \exp\left[\frac{-0.693 \cdot Z \cdot (1 + K_d \cdot P_b)}{t_{1/2} \cdot q}\right] \quad (1)$$

Z = Reference depth (meters).

$K_d = K_{oc} \cdot OC$

K_{oc} = Sorption coefficient. m^3/kg

OC = Organic carbon(OC), fraction(weight basis)

P_b = Bulk density(BD) Kg/m^3

$t_{1/2}$ = Half life of the pesticide (in yrs)

q = Recharge (in meters/yrs).

The reference depth can be either depth to ground water (D2G) or can be the depth at which AF is to be calculated. The weather, soil properties and land characteristics determine the magnitude of q. The net ground water recharge at a site is calculated using the water balance model represented by equation (2).

$$P + I = ET + q + R \quad (2)$$

Where P is the precipitation (cm), I is the irrigation required (cm), ET is evapotranspiration (cm), q is the ground water recharge (cm) and R is the water runoff, on a day d.

In the AFC program it is possible to calculate the AF at any depth below the ground surface or at the end of a soil layer or at the ground water depth. It Fig 1 shows a sample soil profile made up of three soil layers. The data for all the input parameters is available only for the individual layers. In order to calculate the AF for a column of depth d the BD and OC are calculated first, by taking weighted sums of their values at the layers which are above or at the depth d using the following equations

$$BD_d = (BD_{L1} \cdot d_{L1} + BD_{L2} \cdot d_{L2} + BD_{L3} \cdot d_{L3} - d) / d \quad (3)$$

$$OC_d = (OC_{L1} \cdot d_{L1} + OC_{L2} \cdot d_{L2} + OC_{L3} \cdot d_{L3} - d) / d \quad (4)$$

The BD and OC at the D2G can be calculated using (3) and (4) with d equal to depth to ground water. The value of d, however, in this case will be different at different points in the map as opposed to its constant value in previous case.

For calculating AF at the end of a layer L2 the BD and OC can be calculated using the

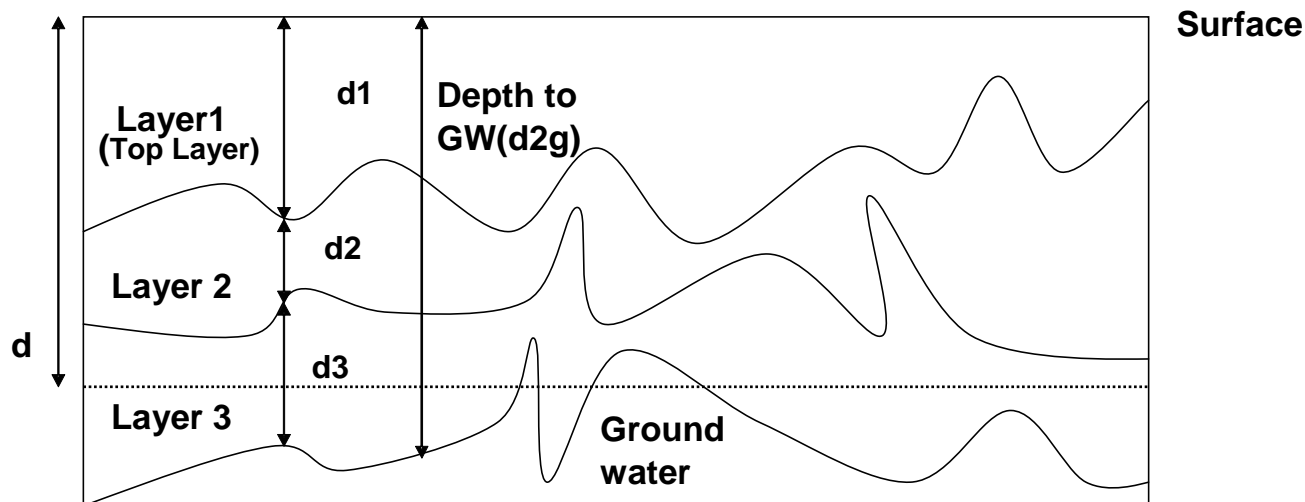


Fig 1. A sample Soil profile

following equations:

$$BD_d = (BD_{L1} * d_{L1} + BD_{L2} * d_{L2}) / d \quad (5)$$

$$OC_d = (OC_{L1} * d_{L1} + OC_{L2} * d_{L2}) / d \quad (6)$$

$$d = d_{L1} + d_{L2} \quad (7)$$

The AF can be calculated using the above weighted values for a given pesticide using (1).

3. Data Formats of Input Files

The inputs to the program are the pesticide information and soil profile information. The pesticide information is provided in the form of an ASCII file with the following format:

Pesticide name Soil half life Sorption

Each of these fields is separated by a tab. The AFC provides a toolbox that helps in generating the file in the above format. Soil profile information is also provided as an ASCII file with the following format

```
SP    site name
# of layers
Filename for RC map            rc
Filename for D2G map           d2g
Filename for Soils map         soils
L    name of layer1 file
L    name of layer2 file
```

The "SP" identifies the file as a soil profile file. The site name is optional and refers to the site or location of study. The next line in the file indicates the number of layers

that the profile contains. This number is used by the AFC to determine if all the layer files are provided; otherwise an error is reported. The next line contains the file name for the recharge map followed by "rc" which identifies it as a recharge map. The D2G map and soils map follows the recharge map entry. These maps are optional. Each of the remaining lines contains an entry for a layer file. Every line is preceded by "L" to indicate that it is a layer file. The layer file is an ASCII file with following format:

<i>File name of map</i>	<i>short description of which parameter it represents</i>
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Keeping the layer information in separate files makes it possible to include different layer files in the soil profile by just changing the name of the layer files it. The input data maps have following ASCII header followed by a binary data of size rows * cols.

```
north: XXXX
south: XXXX
east: XXXX
west: XXXX
rows: XXXX
cols: XXXX
```

The north, south, east and west are not used by the AFC program directly except for writing the output maps. Each cell in the map must contain a real value (single precision floating point) value with the no

data represented as -9999.0. The binary data makes the files smaller in size than their ASCII counter parts and also helps in efficient I/O operations using memory mapped files in JAVA. It is necessary to make the I/O efficient since it is not possible to keep all the data in memory especially in case of large maps. The AFC provides a toolbox which helps in bringing files of different file formats into the AFC native formats. The units of the input parameters should be mutually compatible so that the resulting AF will be unit-less.

4. AFC structure and usage

The program has been written using the J2SDK1.4.1_beta software development kit, which can be downloaded from <http://www.java.sun.com>. Since it is purely written in JAVA it is portable across platforms. However, the platforms on which it has been tested are Windows 2K, XP, 98. Memory space required by the program depends on the size and number of the maps loaded. It is executed by running the batch script provided with the software. The software can be downloaded from the Geospatial Analytics Lab's website of USF, St. Petersburg [4]. The program provides several menu options to make the computation and analysis of the AF easy. Fig 2 shows a snapshot of the program and highlights the main areas. The main menu provides four basic options: *File*, *Compute*, *Filters* and *Toolbox*.

File: This option helps in saving the maps in either an ASCII format through *Export to ASCII* sub-option or in the form of an image through *Export to Image* sub-option. The image can be saved in JPEG or PNG format. The output ASCII file can be saved in the GRASS5 RASTER or ESRI GRID ASCII file formats or in the native AFC format. The native file format is the one in which input files are expected by AFC. The sub-option *Exit* terminates the program. *Load Pesticides DB* option opens a file dialog box to select the pesticides information file and loads the information in the file in the Pesticides Information DIXON_AF_BASIC_FINAL

Panel as shown in the Fig 2. The *Load Soil Profile* loads the soil profile by creating a memory image for all the layers contained in the soil profile. The maps such as recharge, depth to ground water common to all layers are displayed in the display panel under the title "maps common to all layers" as shown in Fig 2. The AFC computes the maximum soil profile depth and sets the upper bound of the slider, in the "Profile Depth Indicator" panel, to this depth. The slider can be used to slice the profile at any depth from 0 to maximum.

Compute: This menu option provides sub-options for computing AF at *selected depth*, *End Of A Layer* or *Depth to ground water*. In case of selected depth and end of layer options it is necessary to select the depth or the layer at the end of which the AF is desired. The depth is selected using the depth indicator slider. It represents variable "d" in (3) and (4). The layer is selected by clicking on one of the radio buttons in the layers panel. This generates the input parameters maps (weighted BD & OM and Depth from Surface) for the given depth or layer. They are shown in the corresponding tabs under the panel named "maps for selected layer/depth". The AF map can be generated by selecting the desired pesticide from the pesticides panel and using the options under the compute menu. The output is shown in the Attenuation Factor tab in the display panel. In case of computing AF with depth to ground water input maps are generated automatically internally and the AF along with the input parameters are shown in their corresponding panels. Each of the generated maps contains a detailed title indicating the layer or the depth for which they are generated. For the AF map the pesticide information is also included in the title. The maps also contain an auto generated legend.

Filters: The AFC allows filtering out values in a map through this option. The AFC provides a very easy way of creating the filters by clicking the right mouse button on the value in the map which is to

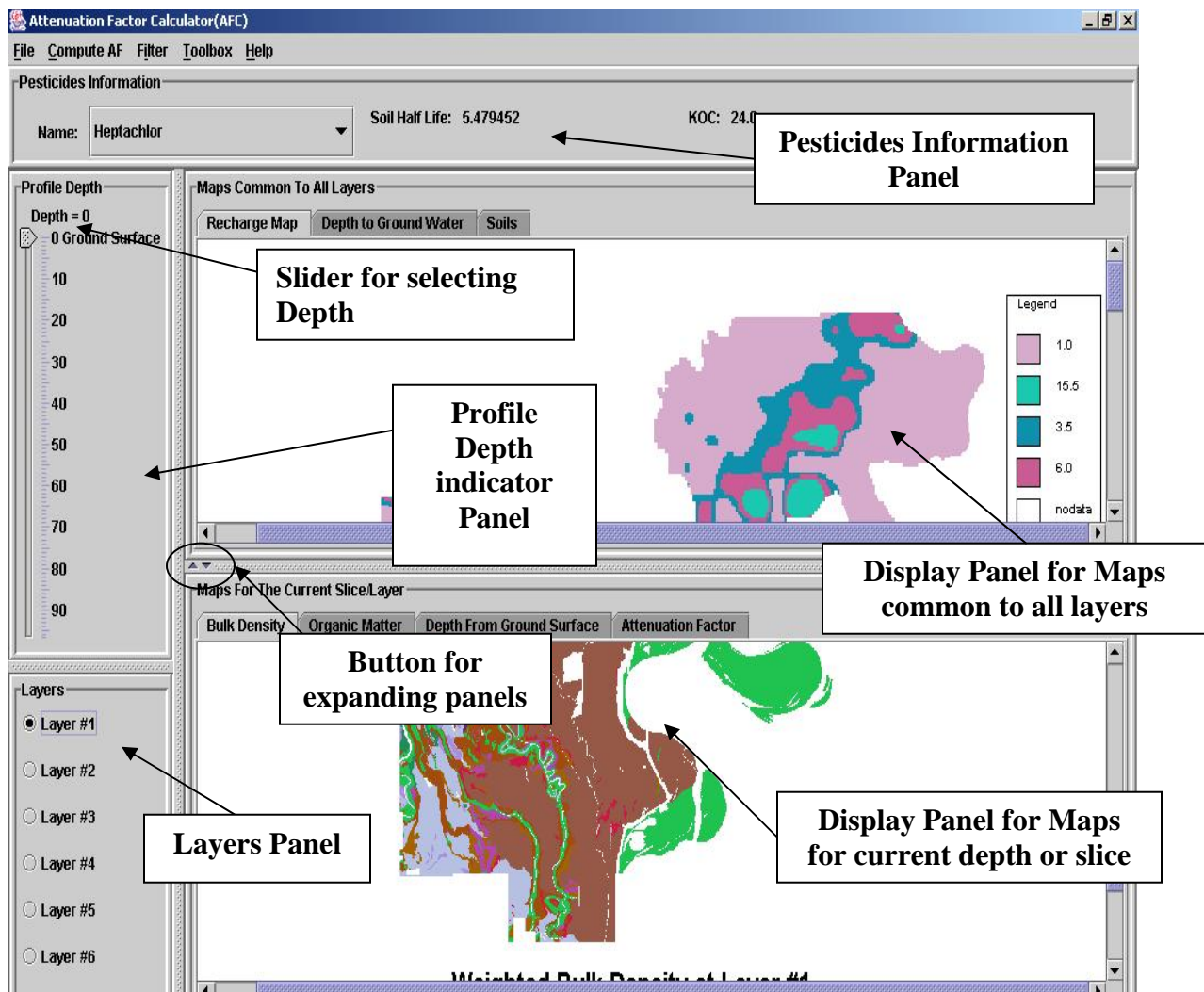


Fig 2. Snapshot of the software showing the main areas

be filtered. This pops up a context-sensitive menu (pop up menu) at the point of the click. It contains sub-options *Create Filter* and *Disable Filter*. The *Create filter* pops up a dialog box indicating the value to be filtered and requires the user to fill the name of the filter which will be used to refer to this filter. AFC ensures that the filter names are unique. A newly created filter is added in the central repository which can be used while applying filters at a later point of time. The *Disable filters* option removes the filter currently applied to a map and brings back the original map. The *Filters* menu provides sub-options *Remove filters* and *Apply Filter*. *Remove Filters* pops up a dialog box containing the names of all the filters created till now.

Filters are removed permanently using this option. The *Apply filter* option pops up a dialog box same as the remove filter option. Applying the filter keeps only the values that satisfy the filter constraints, on the map which currently has the input focus. Filters when applied to a map, on which the filter is not defined, will result in those values, which occur at the same location as the filter value in the map on which the filter is originally defined. For example, if the filter is defined for an AF map on the value of 0.15 and is applied to an OC map, the resulting OC map will contain values which occur at the same location at which the value 0.15 occurs in the AF map. Thus, filters can be used as a query tool and also help in verifying the results.

Toolbox: The menu options under this menu are mainly used to produce files in the format that AFC understands from the user specific data. The *Create Pesticides Database* option creates the pesticides information file in the format required by the AFC. The *Create Soil Profile* option pops up the dialog box shown in Fig 3 (a), (b), (c) which contains input fields for entering the county name, number of layers and the file names of the command maps. To add a layer a “+” button is provided at the bottom. This pops up a dialog box to enter the relevant information. The *Edit Soil Profile* option opens up an existing soil profile file for modification. It has the same GUI as create soil profile but the values are already filled with the values from the profile file to be edited. The Flow Chart for the AFC program is shown in the Fig 4.

Help: This menu provides an option *Help Contents* to open the online manual for the software and the *About* option shows the version and author information.

5. Illustrative Example

The AFC program was tested on the Desha County of Arkansas State. The input data has a resolution of 30 map units, with 2544 rows and 2928 columns. The no data values were represented by -9999. The profile consists of six layers of soil. Average time taken for an operation is 100 seconds and the memory requirements are approximately 700MB. Fig 5 (a), (b), (c) show the BD, OC and Depth from ground surface when the profile was sliced at depth 2 cm. The AF was calculated for pesticide Alachor, with $K_{oc} = 0.00123 \text{ m}^3/\text{kg}$ and half life = 90 days. The output is shown in Fig 5 (d). Figure 5 (e), (f), (g) and (h) show BD, OC, Depth and AF maps at end of layer 2 for the same.

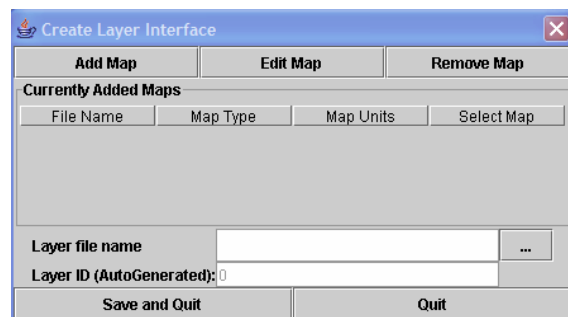
6. Future Work

The software can be extended to support more file formats and provide more analysis tools for verification of the output in the form of graphs, histograms and

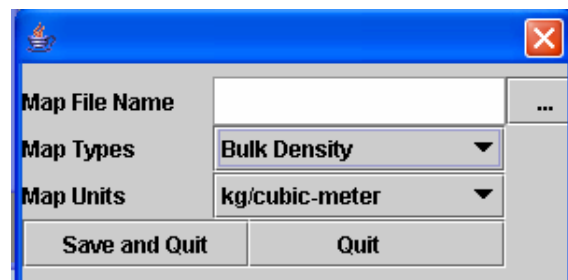
comparison with ground truth. It can be optimized for memory usage and speed to allow faster processing on larger data sets.



(a)



(b)



(c)

Fig 3. User Interface (UI) for soil profile creation (a) UI for adding a layer entry (b) UI for adding a map entry (c) UI for creating a map entry.

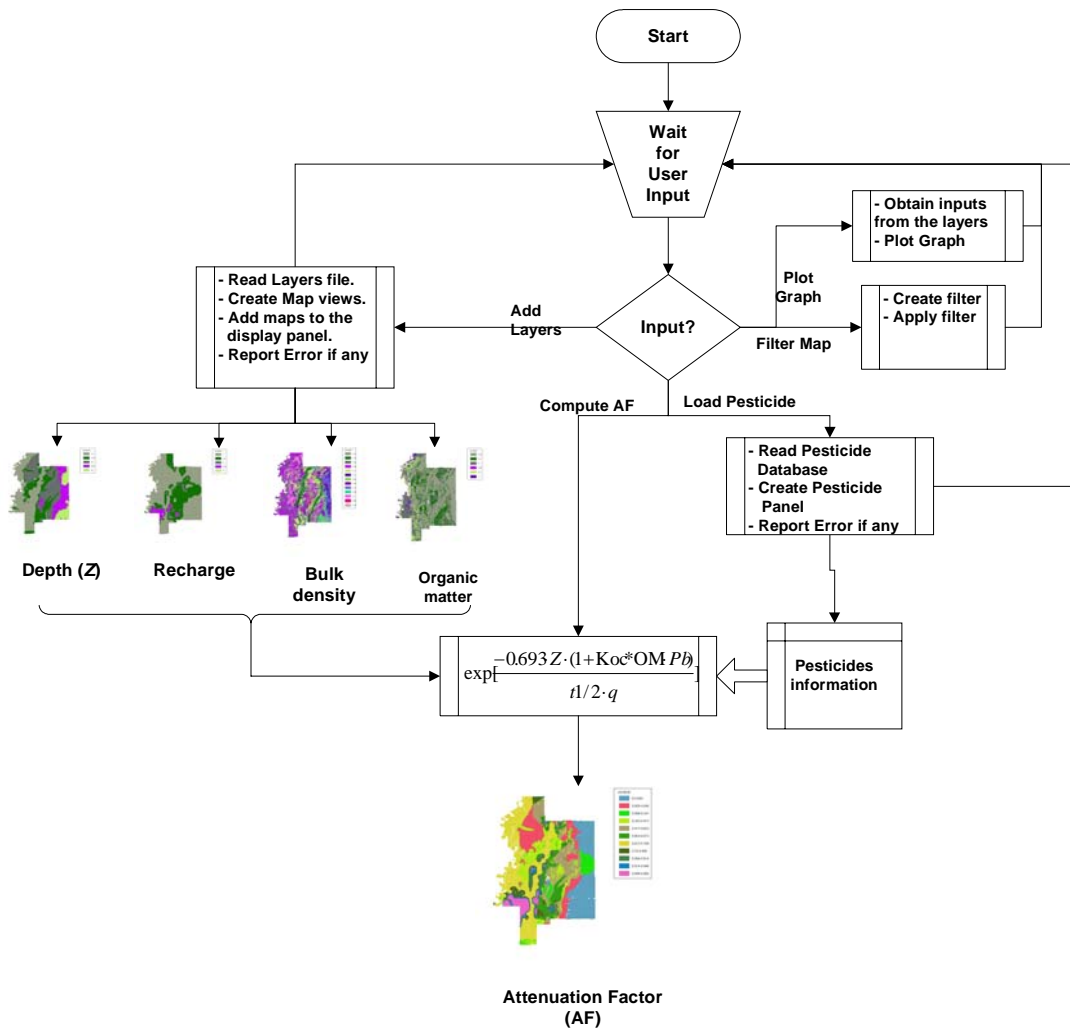


Fig 4. Flowchart of AFC.

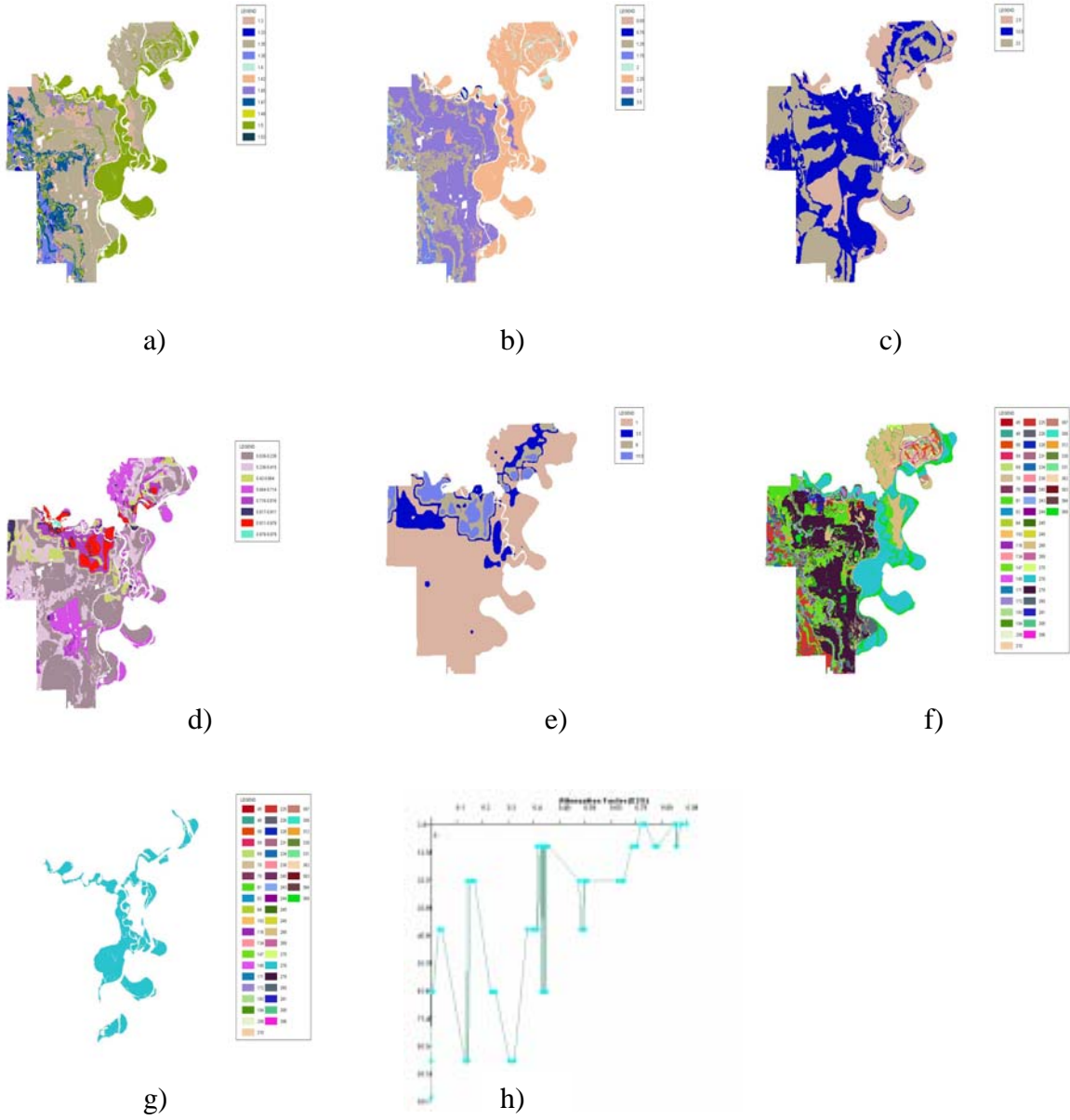


Fig 5. Maps for top layer for Desha County (a) Bulk Density (b) Organic matter (c) Depth to ground water (d) Attenuation Factor (e) Recharge (f) Soils map (g) Soils Map after filtering soil # 276 (h) Variation of AF with D2GW for the top Layer