5. PROCEDURES

This Section describes the procedures utilized to construct the model of agrichemical transport in the Midwest rivers. Section 5.1 shows the steps of preparing published concentrations and flow rate for statistical analysis. Section 5.2 presents Arc/Info procedures that have been prepared to estimate parameters that characterize watersheds within the Upper Mississippi-Missouri River and the Ohio River basins, These parameters include average slope of the rivers, average land slope, distance from the field to the stream along the flow path, exponentially decayed stream length, agrichemical application, average annual temperature, and average annual precipitation depth. Section 5.3 explains the process of converting the database of observations and the sampled watershed characteristic into Splus data objects for further statistical analysis. To make the presentation clearer and more consistent, the detailed description of the statistical analysis is discussed together with presentation of the results in Chapter 6.

Sections 5.4 and 5.5 explain the models of the agrichemical transport in the rivers of the Iowa-Cedar River basin. These models apply results of the statistical analysis of the data that describe the atrazine and nitrate concentrations in the Midwest rivers, the flow rate, watershed morphometry and the climatic parameters. Section 5.4 discusses the method of subdividing the Iowa-Cedar River basin into hydrologic units utilizing a digital elevation model and a digital map of rivers. This section describes also the GIS database of the flow rate and the precipitation depth and the process of the spatial redistribution of the recorded flow rate. The prototype of the agrichemical transport model programmed within the ArcView GIS is presented in Section 5.5.

5.1 Concentration and flow measurements

The data printed in the USGS Open File Report 94-396 (Scribner, et al., 1994) have been manually entered into a computer. The following items have been extracted from the USGS Report: sampling-site name, date of collection (month/day/year), collection time (24-hour), stream-flow (ft³/s), nitrate plus nitrite as nitrogen (mg/L), atrazine ELISA (µg/L), and atrazine GC/MS (µg/L). If more than one sample was taken during one day, the average daily flow-weighted concentration has been calculated as $\overline{c} = \sum_{i} c_i Q_i / \sum_{i} Q_i$ where: c = concentration, Q = flow rate.

The following values have been entered into a computer from the USGS reconnaissance study (USGS Open File Report 93-457, Scribner, et al., 1993): State, site name, date of collection (month/day/year), stream-flow (ft³/s), nitrate plus nitrite as nitrogen (mg/L), atrazine ELISA analyzed in Iowa laboratory (μ g/L), atrazine ELISA analyzed in Iowa laboratory (μ g/L), atrazine ELISA analyzed in Kansas laboratory (μ g/L), and atrazine GC/MS (μ g/L). About 43 missing values of GC/MS atrazine concentration have been determined from ELISA tests using following regression equation that relates ELISA atrazine and GC/MS atrazine (the equation has been estimated utilizing data published in USGS Open File Report 93-457):

$$atrazine = -0.0101 + 0.82547 ELISA + 0.09316 ELISA^2$$
 (5.1)

 $R^2 = 0.92$, 175 observations, Standard Error 0.74 µg/L.

Figure 5.1 shows observed GC/MS atrazine vs. predicted atrazine (Eq. 5.1).



Figure 5.1 Relationship between atrazine ELISA concentration and concentration by GC/MS estimated from data published in the USGS Open File Report 93-457.

The estimation of the CG/MS atrazine concentrations from the ELISA tests is commonly used in practice. Figure 5.2 compares the estimated in this research relationship with the functions developed by different authors.

Thurman et al. (1992) estimated the following quadratic function (Fig. 5.1, line 1):

$$atrazine = 0.21 + 2 ELISA - 0.73 ELISA^{2} + 0.15 ELISA^{3}$$
 (5.2)

 $R^2 = 0.93$, n = 127. It is evident from Figure 5.2 that there is an error in the published equation.

Goolsby et al. (1993) fitted two regression equations for GC/MS values

(Fig. 5.2, line 2 and line 3, respectively), as a function of ELISA values, for samples taken in 1990:

$$atrazine = -0.01 + 0.70 ELISA$$
 (5.3)

 $R^2 = 0.94$; st. error of estimate = 0.09 µg/L, and for samples taken in 1991:

$$atrazine = 0.80 ELISA$$
 (5.4)

 $R^2 = 0.78$; st. error of estimate = 0.10 µg/L

In another study, Moody and Goolsby (1993) estimated the following relationship $(R^2 = 0.94, Fig. 5.2, line 4)$:

$$atrazine = 0.13 + 0.51 ELISA$$
 (5.5)

Gruessner et al. (1995) described the relation between ELISA atrazine and GC/MS atrazine by the equation (5.6):

$$ELISA = 0.029 + 1.16 a trazine$$
 (5.6)

sample size = 217, r = 0.96.

This survey of equations shows that slightly different relationships between CG/MS atrazine and ELISA atrazine are estimated from different data sets.



Figure 5.2 Relationship between atrazine ELISA concentration and concentration by GC/MS estimated by a different authors: (1) Thurman et al. (1992);

- (2) Goolsby et al. (1993) data gathered in 1990;
- (3) Goolsby et al. (1993) data gathered in 1991;
- (4) Moody and Goolsby (1993), and
- (5) relation estimated in this study utilizing data from USGS open file report 93-457.

The streamflow record has been converted from cubic feet per second (ft³/s) into cubic meters per second (m³/s). The two chemical data sets, one from the USGS Open File Report 94-396, and the other from USGS Open File Report 93-457, have been merged and the column containing the site identification number (USGS Station ID) has been added. A simple substitution method (Helsel and Hirsh, 1995) has been applied to values below the reporting limit. For atrazine, 0.025 µg/L replaced a less-then 0.05 µg/L value and for nitrite-nitrate as nitrogen, 0.05mg/L was substituted for a less than 0.1 mg/L value. The summary statistics of the atrazine, nitrite/nitrate-nitrogen concentrations and loads, and the corresponding flow rates are presented in Table 5.1.

	Nitrii	te/Nitrate d	ata set	Atr	azine data s	et
Statistics	Flow	Load	Concentr.	Flow	Load	Concentr.
	m^3/s	g/s	mg/L	m^3/s	mg/s	$\mu g/L$
Mean	82.22	249.8907	5.22	101.15	296.62	5.35
Standard Error	19.20	16.95	0.14	26.82	39.04	0.37
Median	8.85	28.92	2.91	9.72	11.77	1.00
Standard Dev.	694.55	613.18	5.21	819.46	1192.48	11.33
Skewness	22.43	5.43	1.23	19.09	14.06	4.92
Minimum	0.0028	0.0002	0.05	0.0028	0.0011	0.03
Maximum	20416.56	7603.12	26.00	20416.56	27124.85	116.00

 Table 5.1
 Summary statistics of the nitrite plus nitrate and atrazine data sets.

5.2 Preparing data for model parameter estimation

To estimate sampled watershed characteristics, a system of distributed watershed parameters has been developed. This system is composed of a set of grids that describe spatial distribution of such parameters as average agrichemical application rate, average river slope, drainage area, land slope, distance from a field to the river, average annual temperature, and average annual precipitation depth for the Upper Mississippi-Missouri and the Ohio Basins. Each grid cell contains a value that describes a feature of the drainage area upstream of that cell. The 500 m resolution grid, based on the 15 second DEM, is used to accomplish this task. The following factors justify this approach:

- Watershed parameters, that explain the measured loads and concentrations of selected agrichemicals in Midwest rivers, are used to estimate loads and concentrations in unsampled streams;
- Estimating parameters for a region that has area almost 3*10⁶ km², and which is represented by a grid of about 3800 rows and 5800 columns is a

very computer intensive process, so a 100 m cell size would be too intensive;

 A grid-based distributed system of parameters does not require a prior subdivision of region into watersheds nor specification of a watershed outlet.

5.2.1 Preparing 500 m (15") DEM for analysis

The 500 m DEM released by Rea and Cederstrand (1995) has been used in this study. Since it was published using the Albers Equal Area coordinate system with standard projection parameters, no projection was needed.

To ensure that the whole region contributes to the outflow, the DEM depressions must be removed. This is performed by the GRID procedure fill (Listing 5.1, line 1) which produces a "filled" DEM, mwfil, and a grid that contains the flow direction, mwfdr. GRID determines one of the eight directions of the flow from the steepest descent: value 1 represents flow in E (east) direction, 2 in SE direction, 4 - S, 8-SW 16 - W, 32 - NW, 64 - N, and 128 in NE direction. No adjustment of the elevations, i.e., "burning in" RF1 streams has been applied to the 500 m DEM due to the size of the files.

The drainage area upstream of each cell is calculated by summing the number of contributing cells and is calculated by the procedure flowaccumulation(mwfdr), and multiplying by the area of single cell that is equal to a certain value(in this case, 500 m * 500 m = 0.25 km^2 : Listing 5.1, line 2). The stream network is delineated by assuming that a stream is created from the outflow from area at least of 50 km², threshold number of cells (line 3 of Listing 5.1).

The grid function con (*condition*, *true*, *false*) is a conditional statement. The expression *condition* is evaluated for each cell in the analysis window. If it is TRUE, the expression *true* identifies the value to be used to calculate the output cell values. If *condition* is FALSE the output cell is evaluated according to the expression *false*, or, if this expression is not stated, the output cell value is set to NODATA.

Listing 5.1 Creating depressionless DEM, calculating drainage area and delineation of the stream network.

1: fill mwdem mwfil sink # mwfdr
2: mwarea = 0.25 * flowaccumulation (mwfdr)
3: mwstr = con (mwarea > 50, 1)

Before further calculations are made, the stream network delineated from the DEM is compared with the RF1 map to visually verify the flow system. One major inaccuracy was found: the Wisconsin River, a Mississippi River tributary, flowed North to the Great Lakes. To correct this error the elevation of some cells of the DEM were changed to force the flow in proper direction. Correction of the flow system can also be made by making changes directly to the flow direction grid. The process shown in Listing 5.1 was repeated until satisfactory map of the flow system was constructed.

5.2.2 Estimation of watershed parameters

This section presents procedures for estimating the grids which each cell contains the following parameters of the upstream drainage area: average slope of the stream network, average exponent of the stream network length, average distance from field to river, and average slope of the watershed. Slope along the flow path. To estimate the average land slope and the average stream slope, a grid that contains values of the cell slope, measured along the flow path, has to be constructed. Listing 5.2 shows an example of the AML that calculates the slope according to the relation $(H_{i+1} - H_i)/\Delta_L$, where H_{i+1} is the elevation stored in the cell, e.g., mwfil(1,0) pointed by the flow direction grid mwfdr, Hi is the elevation of the processed cell (mwfil), and Δ_L is the distance; cell width (variable %grd\$dx%) or cell diagonal (variable %diag%), depending on the flow direction value. The full listing of the procedure that calculates the slope along the flow path, is presented in Appendix C8.

Listing 5.2 Slope along the flow path.

```
1: &describe mwfil
2: &sv diag = 1.414213562 * %grd$dx%
3: DOCELL
4: if (mwfdr == 1)
     slope3 = ( mwfil - mwfil(1,0) ) / %grd$dx%
5:
    else
6:
   if (mwfdr == 2)
7:
8:
     slope3 = ( mwfil - mwfil(1,1) ) / %diag%
9:
    else
10:
11:
12: . . .
13:
14: if (mwfdr == 128)
15:
     slope3 = ( mwfil - mwfil(1,-1) ) / %diag%
16: else
17: slope3 = 0
18:END
```

Average slope of the stream network. First, the cells that compose the stream network are selected from the grid which contains a description of the direction of flow, mwfdr, - the grid strfdr is created. The number of cells in the upstream stream network is then calculated, using the grid command flowaccumulation.

The same command is used to calculate the sum of the slopes. A grid of average river slope upstream of each cell is obtained by dividing the grid of sum of slopes, slpfacfac, by the grid with the number of cells in the upstream network, strfac. To save disk space, the resulting grid, strslp, is multiplied by 1,000,000 and its values are converted into integer representation. Listing 5.3 shows the GRID dialog which performs this procedure.

Listing 5.3 Average slope of the stream network.

```
1: strfdr = con ( mwstr > 0 , mwfdr )
2: strfac = flowaccumulation ( strdir )
3: slpsfac = flowaccumulation ( strdir, slope3 )
4: strslp = slpsfac / strfac
5: slps6i = int ( strslp * 1000000 )
```

Average exponent of the negative stream network length. According to the information presented in Section 4.3.5 the methodology has been simplified by assuming that the mass that enters the surface waters upstream of each cell is equal to one and is uniformly distributed along the river. The reduced formula describing variable E_s (Eq. 4.9) has the following form:

$$E_{Sk} = \frac{1}{n_k} \sum_{i=1}^{n} \exp(-L_{ik})$$
(5.7)

where:

 E_{Sk} = weighted average of the exponent of negative flow distance in rivers upstream to the *k*-th cell (decay),

 n_k = number of cells that constitute the upstream network (strfac),

 L_{ik} = length of the flow path from the *i*-th stream cell to the *k*-th cell [10² km].

Listing 5.4 shows the GRID dialog for computing parameter E_{Sk} . The command flowlength, that determines the downslope distance along the flow path, from

each cell to the outlet on the edge of the grid, is used to create the grid, mwflg. The exponent of the negative flow distance, expressed in 100 km, is then calculated. The cells that comprise the stream network are selected and the cumulative value of the exponent of the negative flow distance is determined.

Since function flowlength calculates the distance from each cell to the outlet on the edge of the grid, not to the watershed outlet, the grid, strexfac, must be divided by the grid, mwexpflg, according to relation:

$$\sum_{i=1}^{n} \exp(-L_{ik}) = \frac{\sum_{i=1}^{n} \exp(-L_{io})}{\exp(-L_{ko})}$$
(5.8)

where:

- L_{ik} = length of the flow path from the *i*-th stream cell to the *k*-th cell,
- L_{io} = length of the flow path from the *i*-th stream cell to the outlet on the edge of the grid (cell *o*),
- L_{ko} = length of the flow path from the watershed outlet (cell *k*) to the outlet on the edge of the grid (cell *o*).

The division by strfac in line 5, Listing 5.4, is introduced to account for the assumption of a unit mass entering river network. The purpose of the operation stated in the last line of Listing 5.4 is to reduce the size of the computer file; integer grids occupy considerably less disk space than the real-number grids (30%-90% less).

Listing 5.4 Exponentially decaying flow length.

```
1: mwflg = flowlength ( mwfdr )
2: mwexpflg = exp ( -0.00001 * mwflg )
3: mwexpstr = con ( mwstr > 0 , mwexpflg )
4: strexfac = flowaccumulation ( mwfdr , mwexpstr )
5: decay = ( strexfac / mwexpflg ) / strfac
6: decs6i = int ( decay * 1000000 )
```

Average length of the flow path from field to the stream. To exclude the cells that represent a stream network from calculations, a grid containing one in the cells that do not belong to the river network, and zero for the stream cells is created in line 1, Listing 5.5. The downslope distance, along the flow path, from each cell that does not represent a stream to all cells that stand for river is calculated in line 2, Listing 5.5. The average value is determined by summation of all distances upstream (line 3, Listing 5.5) and by dividing the resulting grid, lndflfac, by the total number of cells within the given drainage area that are not streams, lndfac (line 5, Listing 5.5).

Listing 5.5 Average distance from field to a stream.

```
1: lndlstr0 = con ( isnull(mwstr) , 1 , 0 )
2: lndflg = flowlength ( mwfdr , lndlstr0 )
3: lndflfac = flowaccumulation ( mwfdr , lndflg )
4: lndfac = flowaccumulation ( mwfdr , lndlstr0 )
5: alndflg = lndflfac / lndfac
6: alndflgi = int ( alndflg )
```

Average land slope. Listing 5.6, line 1 shows the command used to create a grid, xlndslp, containing the value of the slope in the cells that do not belong to the stream network, and zero for the stream cells. The average slope, lndslp, is calculated by first, summing all of the upstream values of slope, (line 2, Listing 5.6) and by dividing this cumulative slope grid, slplfac, by the total number of cells within the given drainage area that do not represent streams, lndfac, (line 3, Listing 5.6). The last operation converts the slope grid into an integer format.

Listing 5.6 Average land slope.

```
1: xlndslp = con ( isnull ( mwstr ) , slope3 , 0 )
2: slplfac flowaccumulation ( mwfdr , xlndslp )
3: lndslp = slplfac / lndfac
4: slpl6i = int ( lndslp * 1000000 )
```

5.2.3 Creating grid of sampling sites

A grid that represents the USGS sampling sites (watershed outlets) is necessary to extract the parameters of the reconnaissance watersheds from the grids of distributed parameters. This section describes the process used to create such a grid from available data.

The Arc/Info map sta_recon obtained from Battaglin (1995) of 147 sampling sites that are described in USGS Open File Report 93-457 (Scribner, et al., 1993) was converted into raster format by the following GRID operation:

```
sites1 = pointgrid ( sta_recon, station, #, #, 500 )
```

Unfortunately, four of the nine stations from USGS Open-File report 94-396 (Scribner, et al., 1994) are not represented in the sta_recon coverage. Therefore, a coverage of these four sampling sites was constructed from published latitudelongitude coordinates (generate). The attribute table was created (build) and the coordinates of the resulting coverage were changed from geographic projection into Albers projection (project). Finally, this coverage was converted into grid sites2 and merged with grid sites1:

```
site_all = con ( isnull(sites1) , sites2, sites1)
```

The site identification numbers, given in attribute table of the sta_recon coverage (Battaglin, 1995) of the three sites, have been changed to site identifiers that are published in USGS Open-File Report 93-457 (Scribner, et al., 1993), as follows:

```
The Mississippi River at Winfield, ID = 1 has been changed to ID = 05587450
(the Mississippi River at Grafton);
```

The Ohio River near Olmstad, ID = 2 has been assigned ID = 03612500 (the Ohio River near Grand Chain); The Wabash River near Griffin ID = 3 has been replaced by ID = 03378500(the Wabash River near New Harmony).

The drainage area of the original station and the one which replaced it is identical for all three sites.

5.2.4 Adjusting location of sampling sites

The location of most of the sampling sites is not completely consistent with the stream network delineated from the 500 m DEM. Figure 5.3 presents an example of a sampling site (Sta-recon map from Battaglin, 1995) that is located neither on the RF1 stream, nor on the stream network that has been delineated from the DEM.



Figure 5.3 Example of the sampling site (from Battaglin 1995) that is located neither on the stream from RF1 nor on the stream delineated from the DEM.

The cells that represent both the sampling site and the watershed outlet must be located on the proper flow path. The following procedure has been developed to adjust the position of gauging stations:

- constructing a grid of sampling sites that contains published values of drainage area (areap). This step has been performed within ArcView. The new item, dareakm2, has been added to the value attribute table (VAT) of the grid site_all. This VAT is linked to the point attribute table(PAT) of the coverage sta_recon that contains in item darea (the USGS estimates of drainage area in mi²). The values of dareakm2 have been calculated in ArcView using the following formula in "field calculate" entry box: [dareakm2] = [darea] * 2.59, where 2.5900 is the square mile-to-square kilometer conversion factor. The grid, areap, is created from the grid, site_all, by a simple GRID assignment statement (line 1, Listing 5.7);
 - assigning the drainage area value to each cell in the circular neighborhood of cells in grid areap. A five cell radius is assumed (line 2, Listing 5.7);
 - calculating the absolute value of the relative difference between the published drainage area and the distributed values that have been estimated from the DEM in each sampling site cell within its neighborhood (line 3, Listing 5.7);
 - creating grid of zones (zone5) by assigning a unique number to every continuous area with the same value (line 4, Listing 5.7);
 - within each zone, finding a cell that has the smallest difference between the drainage area determined from DEM and the area given by USGS (smallest value in each zone of grid, error5) (line 5, Listing 5.7);

- assigning the site identification number to the cells that have minimum error (lines 6 and 7 of Listing 5.7);
- selecting cells with a relative error of drainage area smaller than 20% (line 8, Listing 5.7)

Listing 5.7 GRID dialog supporting adjustment of sampling sites location.

```
1: areap = site_all.dareakm2
2: usgsarea = focalmax (areap, CIRCLE, 5 )
3: error5 = int ( abs ( ( 100000 * (usgsarea - mwarea) ) /
usgsarea ) )
4: zones5 = regiongroup ( usgsarea, #, FOUR)
5: er_min5 = zonalmin (zones5 , error5 )
6: id_zone = focalmax ( site_all, CIRCLE, 4)
7: siteid5 = con (( er_min5 == error5 ) , id_zone )
8: siteer20 = con ( er_min5 < 20000 , siteid5 )</pre>
```

Wherever possible, the locations of watershed outlets that have a difference in drainage area larger then 20% have been adjusted manually using the grid editor included in ArcTools processor. The results have been stored as mwout grid. About 13% of stations had an error in drainage area larger than 20%. The discrepancies are due to the relatively low resolution of the DEM used in this analysis and, therefore, small precision of the watershed boundaries. These discrepancies are also due to errors in the estimation of drainage area by the USGS. For example, Kalkhoff and Kuzniar (1991) state that the drainage area of sample site 05412100, the Roberts Creek above St. Olaf, Iowa, is equal to 70 mi², whereas Scribner et al. (1993) published a number that is 47% larger (103 mi²). The grid mwout has been used to delineate watersheds from the 500 DEM:

```
mwwsh = watershed ( mwfdr, mwout )
```

Figure 5.4 shows the sampled watersheds delineated from the 500 m DEM.



Figure 5.4 Sampled watersheds delineated from the 500 m DEM.

5.2.5 Extracting parameters of the sampled site watersheds

Listing 5.8 shows the process of extracting watershed parameters from the grids of distributed values and associating them with the site identification number. As a result a VAT is created that contains the following items: mwout (site ID), slps6i2 (stream slope), decs6i2 (decayed flow length), flgl0i2 (flow length from field to stream), and slpl6i2 (land slope).

Listing 5.8 Extracting parameters of the sampled site watersheds.

```
In GRID:
```

```
1: slps6i2 = con ( mwout > 0 , slps6i )
2: decs6i2 = con ( mwout > 0 , decs6i )
3: flgl0i2 = con ( mwout > 0 , alndflgi )
4: slpl6i2 = con ( mwout > 0 , slpl6i )
5: comslps = combine ( mwout , slps6i2 )
6: comdecs = combine ( mwout , decs6i2 )
7: comflgl = combine ( mwout , flgl0i2 )
8: comslpl = combine ( mwout , slpl6i2 )
```

In Arc/Info:

1:	copy coms	slpl comtot				
2:	joinitem	comtot.vat	comflgl.vat	comtot.vat	mwout	mwout
3:	joinitem	comtot.vat	comslps.vat	comtot.vat	mwout	mwout
4:	joinitem	comtot.vat	comdecs.vat	comtot.vat	mwout	mwout

Since the parameters were multiplied by 100000 to convert them to integers, a new Info table that contains the recalculated floating point values has been constructed using Arc/Info and ArcView tools. The items and their units in the new table are as follows: station_id, area (km²), decstr (e^{100km}), slpstr (dimensionless), slplnd (dimensionless), and alflgkm (km). The summary of statistics for a selected parameters of sampled watersheds are presented in Table 5.2. The average land surface slope is approximately one percent while the average stream slope is about six times flatter, or 0.17%.

		Decayed	Stream	Land	Land
Statistics	Area	stream length	Slope	Slope	length
	km^2	E_S	S_S	S_L	$L_L [km]$
Mean	36493	0.59124	0.00168	0.01091	3.34
Standard Error	18360	0.01877	0.00007	0.00057	0.04
Median	1685	0.63221	0.00146	0.00871	3.23
Standard Deviation	224117	0.22912	0.00091	0.00700	0.50
Minimum	173	0.00353	0.00039	0.00130	2.45
Maximum	2335354	0.91928	0.00702	0.04486	5.51

Table 5.2Selected statistics of watershed parameters determined from DEM.Length of the flow path used to calculate E_s is in 100 km.

5.2.6 Agrichemical application

The mass of agricultural chemical that was applied within each watershed in which the concentrations and flow rate were measured, has been calculated using Arc/Info-GRID. This procedure is presented in Listing 5.9. A detailed description of the process is given below:

- In the first four lines of Listing 5.9 the polygon coverages NIT89, NIT90, NIT91, and HERBICIDE1, are converted into grid maps that have cell size equal to 500 m, and grid values equal to the values from items NTOT89.USE, NTOT90.USE, NTOT91.USE, and H1080.USE, respectively. Lines 5-8 transform the application units into grams per square kilometer (g/km²) and modify the format of numbers from double precision to integer to reduce the size of the files. The total application of the nitrogen-fertilizer in all cells upstream of a given cell is calculated in line 9, 10, and 11 for 1989, 1990, and 1991, respectively. The total application of atrazine is determined in line 12.
- The cells that contain the amount of chemical application in the watersheds under investigation are selected in line 13 and they are converted into integer format in line 14 in order to construct a VAT (line 15). The total chemical application map is combined with the grid that contains the site ID number to create a table (VAT) that contains two important items: mwout--the watershed ID and nit89g--the value of chemical use. Lines 13-16 process nitrogen-fertilizer use in 1989. By a similar procedure, the use of the remaining agrichemicals is estimated for each sampled watershed.

Listing 5.9 Chemical application in sampled watersheds.

```
1: xn89 = polygrid(nit89 , ntot89.use, #, #, 500 )
2: xn90 = polygrid(nit90 , ntot90.use, #, #, 500 )
3: xn91 = polygrid(nit91 , ntot91.use, #, #, 500 )
4: xa89 = polygrid(herbicide1 , h1980.use, #, #, 500 )
5: n89gkm2 = int ( xn89 *350262.198 )
6: n90gkm2 = int ( xn90 *350262.198 )
7: n91qkm2 = int ( xn91 *350262.198 )
8: a89gkm2 = int ( xa89 *175.1312741 )
9: n89g = flowaccumulation ( mwfdr, n89gkm2 * 0.25)
10:n90g = flowaccumulation ( mwfdr, n90gkm2 * 0.25)
11:n91g = flowaccumulation ( mwfdr, n91gkm2 * 0.25)
12:a89g = flowaccumulation ( mwfdr, a89gkm2 * 0.25)
13:na89g = con (mwout > 0, n89g )
14:ni89g = int ( na89g )
15:buildvat ni89g
16:comn89 = combine (mwout, ni89g)
```

Table 5.3 shows a summary of the statistics of estimated agricultural chemical use in the sampled watersheds. The application rate has been determined by dividing the total agrichemical application by the drainage area.

	Nitrogen	fertilizer	Atrazine		
Statistics	Application	Appl. rate	Application	Appl. rate	
	kg/yr	kg/km²/yr	kg/yr	kg/km²/yr	
Mean	43705590	5878.1	219644	26.66	
Standard Error	7170678	51.7	40274	0.42	
Median	10298910	6034.0	48695	25.32	
Standard Deviation	259336782	1871.2	1230168	12.74	
Minimum	245134	481.6	466	1.00	
Maximum	4.79E+09	9481.1	19294461	50.55	

Table 5.3Summary statistics of annual application of nitrogen fertilizer and
atrazine.

5.2.7 Annual temperature and annual precipitation depth

Listing 5.10 shows the procedure of creating grids of annual precipitation depth. In line 1 grid prinyr (annual precipitation depth in inches) is created from Arc/Info coverage clim_div, utilizing data stored in its polygon attribute table item pre.mean. Line 2 converts vector map of average temperature (item tmp.mean) into grid representation tmf. In lines 2 and 3 the units are changed from inches to millimeters for precipitation, and from degrees Fahrenheit to degrees Celsius for temperature. Since the Missouri Basin extends behind the US borders, and the clim_div coverage contains data only for the US, temperature of 5 °C (line 4) and precipitation depth of 333 mm (line 3) has been assumed for the Canadian part of the Missouri Basin. A grid of annual precipitation depth in watershed upstream of each cell (prmmavg) is calculated by summing all precipitation-cells over drainage area (line 7, grid mwprfac) and then by dividing the result by the number of cells that constitute upstream drainage area (line 8). The distributed system of the watershedaverage temperature tmcavg is calculated in lines 9 and 10.

Listing 5.10 Average climatic parameters.

```
1: prinyr = polygrid (clim_div, pre.mean)
2: tmf = polygrid (clim_div, tmp.mean )
3: prmm0 = 25.4 * prinyr
4: tmc0 = 5 * (tmf - 32 ) / 9
5: prmm = con (isnull (prmm0), 333 , prmm0 )
6: tmc = con (isnull (tmc0 ), 5 , tmc0 )
7: mwprfac = flowaccumulation(mwfdr , prmm)
8: prmmavg = mwprfac / mwfac
9: mwtcfac = flowaccumulation(mwfdr , tmc)
10:tmcavg = mwtcfac / mwfac
```

The process of extracting temperature and precipitation data for the sampling sites is presented in Listing 5.11. In lines 1-4 the climate grids are converted into

integer format. Before conversion, all grids are multiplied by 1000 to preserve the decimal component (three decimal digits). Lines 5-8 shows constructing grids that contain values only in cells that represent sampled watershed outlets. The VATs that relate sampling site ID stored in grid mwout, and the estimated parameter (command combine) are created in lines 9-12. The summary Info table clim.dat is constructed in lines 13-15. This table contains the following items:

- mwout = sampled watershed ID;
- tcal03s = average temperature over sampled watershed;
- tc103s = annual temperature at sampling site;
- pmma103s = annual precipitation depth, average for sampled watershed;
- pmm103s = annual precipitation depth at sampling site.

The temperature stored in the clim.dat is in 10^{-3} °C and the precipitation depth is in 10^{-3} mm.

Listing 5.11 Creating a summary Info table of climatic parameters.

```
1: pmm1000 = int ( prmm * 1000 )
2: pmma1000 = int ( prmmavg * 1000 )
3: tc1000 = int ( tmc * 1000 )
4: tca1000 = int ( tmcavg * 1000 )
5: pmm103s = con ( mwout > 0 , pmm1000 )
6: pmma103s = con ( mwout > 0 , pmma1000 )
7: tc103s = con ( mwout > 0 , tc1000 )
8: tca103s = con ( mwout > 0 , tca1000 )
9: com1 = combine (mwout , pmm103s)
10:com2 = combine (mwout , tca103s)
11:com3 = combine (mwout , tc103s)
12:com4 = combine (mwout , tca103s)
13:arc joinitem com1.vat com2.vat clim.dat mwout mwout
14:arc joinitem clim.dat com4.vat clim.dat mwout mwout
```

5.3 Preparing data for statistical analysis

The Info tables that contain selected watershed features and annual atrazine and nitrogen-fertilizer application have been merged with the table that contains measured flow and concentration in 153 sampling sites on the Midwest rivers. Two tables have been created: atra7 and nitr7. The table, atra7, contains the following data:

	atra7		nitr7
state	state name abbreviation	state	state name abbreviation
name	name of the sampling site;	name	name of the sampling site;
id	station id;	id	station id;
area	drainage area in km ² ;	area	drainage area in km ² ;
use	total mass of atrazine use in kg/yr;	use	total mass of N-fertilizer use in kg/yr;
appl	atrazine application rate in	appl	nitrogen-fertilizer application rate in
	kg/km²/yr;		kg/km ² /yr;
date	month/day/year of sample collection;	date	month/day/year of sample collection;
day	day in which sample was collected,	day	day in which sample was collected,
	1365;		1365;
month	month in which sample was	month	month in which sample was
	collected, 1-12;		collected, 1-12;
flowm3s	flow rate in m^3/s ;	flowm3s	flow rate in m^3/s ;
loadmgs	atrazine load in g/s;	loadgs	nitrate load in g/s;
loadgd	atrazine load in g/d;	loadkgd	nitrate load in kg/d;
concmgm3	concentration in $\mu g/L$ (mg/m ³⁾ ;	concgm3	concentration in mg/L (g/m^{3}) ;
decstr	exponent of negative flow length;	decstr	exponent of negative flow length;
decInd	exponent of negative distance from	decInd	exponent of negative distance from
	field to stream network;		field to stream network;
slpstr	slope of the streams;	slpstr	slope of the streams;
slpInd	average slope of the land;	slplnd	average slope of the land;
alflgkm	average length from field to stream	alflgkm	average length from field to stream
	network in km;		network in km;
prmm	precipitation at sampling site mm/yr	prmm	precipitation at sampling site mm/yr
prmmavg	precipitation depth in sampled	prmmavg	precipitation depth in sampled
	watershed mm/yr		watershed mm/yr
tmc	annual temperate at sampling site °C	tmc	annual temperate at sampling site °C
tmcavg	average temperature in sampled	tmcavg	average temperature in sampled
	watershed °C		watershed °C

Table 5.4Description of tables atra7 and nitr7.

The statistical program Splus operates only on objects. All data and results of statistical analysis are stored as objects. A table can be stored as an *array* object or as a *frame* object. The atra7 and nitr7 data sets have been imported into Splus data object *frames*:

```
atra7 _ read.table("atra7" , header=T)
nitr7 _ read.table("nitr7" , header=T)
```

Stepwise regression has been used to estimate model parameters. The following commands show an Splus session for selecting significant components of the model by the stepwise regression:

```
alnc.lm _ lm(log(concmgm3) ~ 1, data = atra7)
acla _ step(alnc.lm, ~ log(appl) + log(flowm3s)
            + log(decstr) + slpstr
+
            + log(alflgkm) + log(slplnd)
+
            + month + sin(pi*month/12) + cos(pi*month/12)
+
            + sin(2*pi*month/12) + cos(2*pi*month/12)
            + sin(4*pi*month/12) + cos(4*pi*month/12)
+
+
           + sin(6*pi*month/12) + cos(6*pi*month/12)
           + sin(8*pi*month/12) + cos(8*pi*month/12)
+
            + sin(10*pi*month/12) + cos(10*pi*month/12)
+
            + sin(12*pi*month/12) + cos(12*pi*month/12) )
```

The results of regression analysis are displayed by the Splus command summary ()

```
summary (acla)
```

Different models have been tested by adding or removing model components. The following line shows removing variable log(appl) from the model acla:

acla2 _ update(acla, . ~ . - log(appl))

Two diagnostic plots have been used to visually validate the assumption that the residuals are normally distributed:

1) plot of residuals versus fitted values

```
plot(fitted(acla), studres(acla) )
```

2) a normal quantile plot of residuals

```
qqnorm(resid(acla))
qqline(resid(acla))
```

The data can be transformed within the specification of the regression model, as well as the new columns in the data frames can be derived from the original data set. Below are two examples of creating new values from existing ones:

```
nitr7[,"srslpstr"] _ sqrt ( nitr4[,"slpstr"] )
nitr7[,"etstr"] _ nitr6[,"decstr"] ^ ( 1 / nitr7[,"srslpstr"] )
```

The results of the statistical analysis of data and the agrichemical transport models selection are discussed in Chapter 6.

5.4 Agrichemical concentrations in the lowa-Cedar River basin

The procedure of modeling of agricultural chemical concentration and load in the Iowa River and its tributaries includes:

- The Iowa-Cedar River basin is subdivided into modeling units, using the 100 m DEM. This step includes such operations as downloading 1° DEMs via Internet, converting the RF1 river map from vector format to raster format, determining a map of the flow direction, creating a map of the USGS gauging stations, constructing a map of modeling unit outlets, and determining modeling unit boundaries;
- The map of modeling units is converted from grid into vector format;

- The parameters of the total drainage area that is defined by the outlet point of the modeling unit, such as average distance from the field to the stream, and watershed slope, are estimated from the 100 m DEM, and inserted into modeling unit polygon attribute table;
- The mean monthly runoff at each outlet of the modeling unit is calculated, utilizing the measured runoff in 28 USGS gauging stations and observed precipitation depth from 86 NCDC stations;
- The link between map of counties that contain data about the agrichemical application and the map of unit watersheds is established;
- The equation that describes the concentration of agrichemicals in streams is incorporated into the GIS database;
- For each spatial unit and each month of the year, a regression equation is applied to calculate chemical concentration at the elementary watershed outlet;
- The spatial distribution of chemical loads is estimated by multiplying the concentration by the mean monthly flow rate at each outlet.

5.4.1 Creating a map of the flow direction

Downloading DEM via Internet. Nine, one-degree quadrangles (mason city-w.gz, mason city-e.gz, waterloo-w.gz, waterloo-e.gz, dubuque-w.gz, des moines-w.gz, des moines-e.gz, davenport-w.gz, and davenport-e.gz) of DEMs that contain digital elevation data for the region enclosed by meridians: 90° and 94° West (longitude) and by parallels 41° and 44° North (latitude), have been downloaded from the USGS National Geospatial Data Clearinghouse via Internet

(http://edcwww.cr.usgs.gov/glis/hyper/guide/1_dgr_dem). Figure 5.5 shows the location and the names of the downloaded quadrangles.



Figure 5.5 1° quadrangles of DEM utilized to subdivide the Iowa-Cedar River basin into modeling units; Map projection: geographic.

The files have been uncompressed (UNIX command gunzip), and modified as explained below. The DEM files do not contain record delimiters, thus they should be added by the following UNIX command:

dd if=inputfilename of=outputfilename ibs=4096 cbs=1024 conv=unblock

No direct conversion of the USGS DEM's into Arc/Info GRID format is supported. The Arc command demlattice has been used to convert a DEM in USGS or TAME format into a lattice. The following example shows the conversion of the DEM waterloo_e.dem into Arc lattice us4292lat: Arc: demlattice waterloo_e.dem us4292lat USGS

After all nine DEMs were converted into lattices, they were merged to construct a single map. For example, the following grid command has been used to merge four lattices:

Grid: crlat1 = merge(us4394lat, us4393lat, us4294lat, us4293lat)

In Arc/Info, the concepts of lattice and grid are similar, with one important exception. A lattice is a regularly-spaced sample of points representing a surface. Elevation values in a lattice correspond to discrete points. In a grid, the values apply to the entire cell. Although both lattice and grid apply the same data structure, the fact that a lattice represents data at points (has no area) and grid cell has an area, causes differences in how various operators interpret the data contained in a lattice and within a grid. The further analysis described here, in which the lattices were treated as grids, was not affected by these differences.

Since imported maps are in geographic coordinate system (latitude/longitude) they have been projected into Albers system (project), assuming the cell size of output grid equal to 100 m. Appendix C9 contains a macro that converts a grid into Albers Equal Area coordinates. The following parameters have been used:

Units METERS Datum NAD83 Spheroid GRS1980 1st standard parallel = 29 30 0.000 2nd standard parallel = 45 30 0.000 central meridian = -96 0 0.000 latitude of projection's origin = 23 0 0.000

Converting river map from vector format into grid representation. The following GRID commands have been applied to specify the cell size and the map extent of the rasterized RF1:

```
setcell crdem
setwindow crdem
```

The portion of the RF1 map that represents rivers in the Iowa-Cedar River basin has been converted into grid format by applying the linegrid command:

```
crrf1 = linegrid ( rf1, rf1_id )
```

The item, rf1-id, from the AAT (arc attribute table) has been used to assign values to the cells that represent rivers. This item has been selected since it allows one to relate the grid VAT table with the RF1.FLOW Info table, through one of the following identification fields: CUSEG (hydrologic cataloging unit code and reach segment number) or RR (Reach File ID --an unique identifier for each river reach). The table, RF1.FLOW, contains useful information for hydrologic modeling. For example, it comprises such items as: LFVEL--low flow velocity, MFVEL--mean flow velocity, MNFLO--USGS mean annual flow, and SVTEN--USGS 7-10 Year Flow (Lanfear, 1994).

The raster version of RF1 was edited using Arc/Info interactive editing environment, arctools. The lakes were replaced by a single line or, if the region of lake was enclosed, by the series of cells that fill up the enclosed region. The resulting data set was saved under the original grid name, crrf1.

Creating a map of the flow direction and delineation of the stream network.

To ensure that the flow paths delineated from the DEM are in line with the RF1 river network, the terrain map has been adjusted. Elevations of all cells that do not represent the real stream network have been raised by 10000 m:

```
crdem2 = con ( isnull ( crrf1 ), crdem + 10000 , crdem )
```

The value 10,000 was selected arbitrarily. During this research it was found that this increment should be larger than the maximum elevation of the DEM within the analysis region for two reasons:

- To ensure that the cells that constitute the stream network are lower than the cells that do not represent the stream. For example, increasing the elevation of all cells that do not represent the stream network by 5 m in the DEM which values vary from 0 to 50 m does not ensure the stream-cells to be below the neighboring land-cells (except for smoothed DEMs). Thus an uncertainty about the compatibility between RF1 rivers and the delineated rivers is introduced;
- 2) To easily select all cells that have been adjusted. Selection can be made by a single conditional grid expression, for example, all adjusted cells in grid crdem2 can be set to 1 by the following grid assignment:
 output = con (crdem2 > 9000 , 1).

The depressions have been removed to ensure that the whole region contributes to the runoff, and the flow direction grid crfdr has been built:

```
fill crdem2 crfill2 crfdr
```

Rivers have been delineated under the assumption that the runoff from a drainage area of 25 km² produces a stream. To all cells that have an accumulated number of cells greater than $2500 (= 25 \text{ km}^2 \text{ with } 100 \text{ m DEM cells})$ "flowing" into them, the value one has been assigned:

```
crfac = flowaccumulation ( crfdr)
crstr25 = con ( crfac > 2500 , 1, 0)
```

Conversion of the RF1 file into a 500 m by 500 m raster format revealed that the cell size of 500 m is too large to represent 1:500,000 river network, without

ambiguity. Some of RF1 reaches are closer to each other than one kilometer, and if converted into 500 m grid they are artificially connected. When applied in the procedure described above, i.e., if the RF1 streams are burned into the 500 m DEM, these connected rivers cause the GRID command flowdirection to determine a false direction of flow (due to the difference in elevation of watersheds). As a result, the water flows from one watershed into another through connected streams that belong to different basins. Figure 5.6 shows the low precision of the streams delineated from 500 m DEM adjusted for RF1 streams. The same streams but delineated from a 100 m DEM adjusted for RF1 almost perfectly represent the RF1 rivers--this justifies the application of the 100 m DEM in this study.



Figure 5.6 Comparison of the stream network delineated from 100 m DEM (a) with the one delineated from 500 m DEM (b). Both DEMs were adjusted for RF1 stream network.

5.4.2 Map of the modeling unit outlets

A watershed is explicitly defined by its outlet point. Therefore, to subdivide the basin into elementary watersheds, a set of points -- elementary watershed outlets-must be specified. Three types of watershed outlets are utilized to subdivide the Iowa-Cedar River basin into units:

- The most upstream cell of the first order stream;
- The most downstream cell of each reach; and
- The cells that represent the USGS stations.

Figure 5.7 shows examples of watershed outlets



- Figure 5.7 Selected types of the modeling unit outlets (a) type 1, beginning of the stream network; (b) type 2, upstream cell of the stream junction; (a) type 3, USCS gauging station
 - (c) type 3, USGS gauging station

Beginnings of the delineated stream network (type 1 outlets). As was mentioned in Section 4, the type 1 outlets have been introduced to have more control on the average area of the modeling unit and to determine the flow (and chemical load) conditions at the beginning of the river system. Listing 5.12 shows the Grid dialog that selects appropriate cells. In line 1, the raster stream network crstr25 is divided into "grid zones" crls1. In Arc/Info GIS a grid zone is developed from the cells that have the same value. Command streamlink assigns an unique value to each stream reach. In line 2, zonalmin function finds the minimum value in flowaccumulation grid crfac delineated by the zones of crlsl and assigns it to all cells of the reach. Function streamorder (line 3) assigns to each reach a numeric order (Strahler or Schreve). In line 4, the most upstream cell in the first order stream is found by selecting the cell that has the same value in both grids, crlmn and crfac. The value of the selected cells is equal to the value from the grid crisi increased by 100,000, to indicate the type 1 outlet and thus the type of watershed (source watershed). This number also indicates (after subtracting 100,000) the ID of the downstream unit (intermediate watershed) making the numbering system of the hydrologic structure consistent and efficient.

Listing 5.12 Selecting type 1 watershed outlets.

```
1: crlsl = streamlink ( crstr25 , crfdr )
2: crlmn = zonalmin (crlsl , crfac )
3: crlso = streamorder ( crstr25 , crfdr )
4: crlpu = con(crlso == 1 AND crlmn == crfac, crlsl + 100000)
```

River junctions (type 2 outlets). The type 2 outlets are determined by selecting the most downstream cell in each stream reach. The selection is made by finding in each "grid zone," defined by grid crsls, a cell that has the maximum value in

flowaccumulation grid crfac (Listing 5.13). The last operation shown in Listing 5.13 merges the grid of type 1 outlets with the grid of type 2 outlets.

Listing 5.13 Selecting type 2 watershed outlets.

```
1: crlmx = zonalmax (crlsl , crfac )
2: crlpd = con(crlmx == crfac, crlsl)
3: crlud = con ( isnull( crlpu), crlpd, crlpd)
```

USGS gauging stations (type 3 outlets) The description of the USGS gauging stations published by Hydrosphere (Hydrosphere, 1994) contains latitude and longitude. These coordinates have been used to produce a point coverage of the USGS stations (Listing 5.14). Listing 5.15 shows a part of the file, latlonfl.csv, that contains point coordinates.

Listing 5.14 Creating point coverage of gauging stations from latitude-longitude coordinates.

```
Arc: generate xgsflow
Generate: input latlonfl.csv
Generate: points
Generate: q
Arc: build xgsflow point
```

Listing 5.15 Fragment of the file latlonfl.cvs containing station IDs and coordinates.

5448500,-337370,154670 5449000,-337051,154831 5449500,-337056,153936 5451700,-334285,151225 . . .

To make the point coverage compatible with other maps used in this study, it has been projected into Albers system of coordinates as follows (Listing 5.16):

Listing 5.16 Projecting the point coverage of USGS gauging stations from Geographic system into Albers coordinates.

```
Arc: project cover xgsflow gsflow
Input
Projection geographic
units ds
Parameters
output
Projection ALBERS
Zunits
            NO
Units 

Spheroid GRS1980

W-bift 0.000000000
             0.000000000
Yshift
Parameters
 29 30 0.000 /* 1st standard parallel
 45 30 0.000 /* 2nd standard parallel
-96 0 0.000 /* central meridian
 23 0 0.000 /* latitude of projection's origin
0.00000 /* false easting (meters)
0.00000 /* false northing (meters)
end
```

The grid representation of the USGS stations that is compatible with the delineated stream network has been developed using Arc/Info grid editor tools (arctools). The following line combines the grid with the USGS stations crgs with the grid of watershed outlets crlud:

```
crout = con ( isnull( crlud), crgs, crlud)
```

Since the gauging station cells may overlap with other cells representing watershed outlets units the following statement can be used to establish the priority of which cell needs to be selected in the final map of the modeling units (grids priority from the highest to the lowest: crlpu, crgs, crlpd):

```
crout = con( isnull(crlpu) , con( isnull(crgs), crlpd, crgs), crlpu)
```

The map of modeling units is created by the following Grid statement:

```
crwsh = watershed (crfdr , crout)
```

An Arc/Info script has been developed to create the following grids: stream network, watersheds, and watershed outlets. The complete listing of this program, wshgs.aml, is presented in Appendix C1. A first order watershed, and its outlet cell, have an ID number in the range 100000 < ID < 200000. This number is the ID of the first order stream increased by 100000. A watershed that drains through the point at which the gauging station is located assumes the USGS gauging station identification number, 5448500 for example.

5.4.3 Watershed connectivity

To determine the average value of the model parameters for the drainage area upstream of a given point, the sum of values for all upstream modeling units must be calculated. All these units can be identified if the position of each unit on the flow path is known. The Arc/Info script nextwsh.aml creates an Info file with two items that store the modeling unit ID number and the ID number of the next unit on the flow path (downstream unit). The listing of the macro nextwsh.aml is shown in Appendix C2. The major part of this AML assigns to the cell that corresponds to the watershed outlet crout a value from the cell, located in watershed grid crwsh, that is pointed by the flow direction crfdr. In line 1, Listing 5.17, a value zero is assigned to all cells that have NODATA (xcrwsh). This step is necessary to ensure that the next watershed to the last unit on the flow path is indicated by the ID equal zero (no downstream units). Lines 2-9 create a grid crnxt similar to the grid of watershed outlets crout but with ID of the downstream unit.

Listing 5.17 Identification of the downstream watershed ID.

4:	$con (crfdr == 4, xcrwsh(0,1), \sim$
5:	con (crfdr == 8, xcrwsh(-1,1), ~
6:	con (crfdr == 16, xcrwsh(-1,0), ~
7:	con (crfdr == 32, xcrwsh(-1,-1), ~
8:	con (crfdr == 64, xcrwsh(0,-1), ~
9:	con (crfdr == 128, xcrwsh(1,-1), -1))))))))

5.4.4 Refining modeling units

Two problems occurred when the grid of modeling units was converted into vector format:

- Small zones were not converted into visible polygons, although the records in polygon attribute tables were created. This makes it impossible to select records in the PAT by pointing to polygons on the screen;
- 2) A simple grid zone had more than one component area and the components were connected by the cell corner. It was converted into more than one polygon, i.e., one modeling unit was described by two records in the PAT. For this unit, the value that represents an area in the VAT, after conversion into a polygon coverage, was listed in the PAT twice. Thus, the modeling unit had two times larger area in vector map than the same unit represented in the grid.

To solve the problems mentioned above, all zones of smaller area than one km^2 (1 km² = 100 cells 100 m * 100 m) were incorporated into neighboring units. The GRID nibble command replaces areas in a grid corresponding to a mask with the values of the nearest neighbors (Listing 5.18):

Listing 5.18 Eliminating drainage units that are smaller than 1 km²

```
aaa = crwsh.count
aaa2 = con (aaa > 100 , 1 )
crwsh2 = nibble(crwsh, aaa2, DATAONLY )
```

The nibble command has also been used to remove the upstream portion of the unit composed of two parts connected only by the cell corner.

The removal of small drainage areas introduced discontinuity of the flow system. A program was written in C language to determine the new relation between modeling units. The C code of the program newnx.c is listed in Appendix A1. This procedure requires two text (ASCII) files. In the first file, each line contains two numbers separated by a comma: unit_id and the downstream unit_id, for the original set of modeling units. The second file contains only the list of unit_id --identification numbers of units that remained from the original set after some of them have been removed. Program newnx creates an ASCII file in which it stores updated information about system connectivity. In each line, the following numbers are written, separated by a comma: unit_id, downstream unit_id, and numeric order of the unit in the flow system.

By assigning a numeric order to each unit, the further calculations are more efficient. The method of stream numbering is as follows: all exterior units, i.e., the most upstream units are assigned an order 1. The order of each interior unit is calculated as the maximum order of the upstream units increased by one.

The advantage of the program written in C over the procedure written in Arc/Info macro language or in ArcView script language Avenue, is that the C program, after minor changes, can be used by both Arc/Info and ArcView, whereas program written in AML can be executed only from Arc/Info, and a script written in Avenue language can only be run from ArcView. The additional advantage of writing more complex procedures in such languages as FORTRAN or C is that the time of execution is very fast. The time gain is on the order 1000, i.e., the computational hours can be reduced to seconds. The following assignment creates the final map of the modeling units in vector format (weed tolerance = 180 m):

crwsd = gridpoly (crwsh3 , 180)

The map of subdivision of the Iowa -Cedar River basin into 1032 modeling units is presented in Figure 5.8.



Figure 5.8 The Iowa-Cedar River basin subdivided into 1032 unit drainage areas of average area 31.6 km².

5.4.5 Database of monthly precipitation depth and monthly flow rate

The time series of the average monthly flow rate and the average precipitation depth for 38 USGS gauging stations and 86 climate stations, for the time period from January 1940 to September of 1992, have been extracted from the Hydrosphere CD-ROMs (Hydrosphere 1993 a, b) and stored in a worksheet format.

The units of measurements have been changed:

- cubic feet per second (cfs) into cubic meter per second (m^3/s) (flow) and
- inch per day into centimeter per day (cm/d) (precipitation).

For each parameter, two sets of ASCII comma delimited files have been created. One set contains identification numbers of observation stations and respective longitude and latitude, expressed in decimal seconds. The other set of files comprise the station ID number and the time series of flow or precipitation.

The point coverage of 86 precipitation stations has been created from the ASCII files and projected into Albers Equal Area system of coordinates. This procedure is identical to the one described in a previous section for generation of point coverage of USGS stations.

The ASCII files that contain flow and precipitation measurements have been converted into Arc/Info INFO files and linked with the appropriate maps.

5.4.6 Average precipitation depth in modeling units

The method of spatial redistribution of measured flow rate utilizes the precipitation depth as a weighting factor. Therefore, the monthly average precipitation depth must be calculated for each modeling unit. The example of the GRID dialog which calculates a raster map of the average precipitation depth, in modeling each modeling unit for May 1990 is shown in Listing 5.19.

The grid of distributed precipitation depth has been created directly from the climate station map. The inverse distance weighting procedure iwd has been applied. To make the calculations shorter and to save the disk space, 100 times larger cells (width = 1000 m, area =1 km²) than those used for the stream and modeling unit delineation have been assumed (setcell 1000). The average values for each modeling unit have been determined by the zonalmean function. To create an attribute table, the cell values must be represented as integers. In line 7 of listing 5.19, the grid, xxx1, that contains zonally averaged precipitation depth is first multiplied by 10000 to preserve the decimal part and then converted into integer format. The command combine has been used to create a table in which the modeling unit identification number (stored in grid crwsd) is related to the estimated average precipitation depth (stored in grid xxx2).

Listing 5.19 Estimation of the average precipitation depth in modeling units.

```
1: setcell 1000
2: setwindow MAXOF
3: xxx = idw ( gsrain , m199005 )
4: setcell crwsd
5: setwindow crwsd
6: xxx1 = zonalmean ( crwsd , xxx )
7: xxx2 = int ( 10000 * xxx1 )
8: xxxcom = combine (crwsd, xxx2)
```

Since the procedure described above must be executed for each month, it has been included into AML's DO feature that repeats calculations for each month of the specified time period,. i.e., from month %fm% of the year %fy% to month %tm% of the year %ty%. An example of the &DO block is presented in Listing 5.20

Listing 5.20 Application of the &DO command to repeat action for each month of the selected time period.

```
1: &DO yr = %ty% &to %fy% &by -1
2: &DO mt = 12 &to 1 &by -1
     &s ab = [calc %yr% = %fy%] AND [calc %mt% lt %fm%]
3:
     &s bb = [calc %yr% = %ty%] AND [calc %mt% gt %tm%]
4:
5:
     &s cc = %ab% OR %bb%
     &IF NOT %cc% &THEN
6:
7:
        ob&
           . . . /* here, block to be repeated
8:
9:
        &end
10:
     &end
11:&end
```

Appendix C3 contains the code of the Arc/Info macro RAININFO.AML. This program calculates average values for specified zones and then writes them into an INFO file. The user must specify the period for which the estimates have to be made, the point coverage that holds the time series, and the grid that divides the region into zones. The output of the macro is the Arc/Info INFO file that contains for each zone the ID number and the series of computed zonal averages.

In the approach presented above, only stations that have complete time series, i.e., stations that have no missing values, have been applied. The macro SELDATA.AML that is included in Appendix C6 selects stations that have a complete record in the specified time interval.

To include all available measurements of precipitation depth, another approach has been tested. The stations that have data for the processing month have been used, unlike the method discussed above in which only the stations that have data for all months of the specified time period have been utilized. For each month, station selection is performed (Arc/Info command reselect) and then the grids of spatial distribution of the precipitation depth are calculated (IDW procedure). This task is performed by the macro RAINMAP.AML (attached in Appendix C4). The results were slightly different, but since the zonal averages were calculated later, the differences were insignificant. Listing 5.21 shows an example procedure that selects all stations from the database (coverage prcmap) that have a complete record in June, 1966 (point coverage xxx), and then it creates the grid of precipitation (pm196606) by the inverse distance-squared method:

Listing 5.21 Example of the AML that selects precipitation stations that have a complete record in June, 1996 and creates the grid of precipitation depth (adopted from RAINMAP.AML).

```
1: arc reselect precmap xxx point
2: res m196606 ge 0
3: ~
4: n
5: n
6: arc build xxx point
7: pm196606 = int ( 1000 * idw ( xxx, m196606 ) )
8: kill xxx all
```

5.4.7 Spatial distribution of flow

Three approaches have been made to incorporate the procedure described in Section 4.5 into GIS. Coding has been made in:

- 1) Avenue, the script language of ArcView;
- 2) Arc/Info macro language, AML;
- 3) C programming language.

For the first two approaches, the calculations of the flow rate for a single month took hours, whereas the program written in C language redistributed the flow record in a few seconds. Therefore a method that uses the Arc/Info Tables to prepare the data and then utilizes the C program to calculate the flow rate in modeling units has been developed. It is explained here for a single month: March 1990. The full Arc/Info macro--fd4y.aml--is presented in Appendix C7. The C program-fd4y.c--is listed in Appendix A2. The fd4y program requires two input files and it stores the results in one output file. In lines 2 and 3 of Listing 5.22, the Arc/Info processor, Tables, creates the first input file xxxgsin in which the following items of the point attribute table gsfl28.pat are stored:

- station_id = ID number of the USGS gauging station;
- station_nx = ID number of the downstream USGS station;
- m199003 = item that contains flow record for March 1990

The second input table, xxxunin, is prepared in lines 4 and 5. The following items are unloaded from the polygon attribute table unprec.pat:

- unit_id = modeling unit ID number;
- unit_nx = ID number of the downstream unit
- gswsh = ID of the USGS gauging station that is located downstream from the given unit;
- area_km2 = area of the unit;
- order = modeling unit order in the flow system; and
- pm199003 = item that contains average precipitation depth.

The program fd4y is executed in line 6. Since UNIX is a multitasking system, the AML must wait until fd4y finishes calculations. Lines 7 to 10 contain the loop in which AML checks if fd4y program created output file xxxunout. In lines 11 to 14, the temporary INFO file m199003.dat is created in which the results of the fd4y calculations are stored (line 15). Then, the estimated flow rate is attached to the Arc/Info database file unflow.pat (line 17) and the temporary file m199003.dat is deleted (line 18). In the complete version of this procedure (fd4y.aml), the process described here is repeated for all months of the specified time period. Figure 5.9 presents an example of estimated runoff that occurred in June 1990.

Listing 5.22 Example of the Arc/Info macro that prepares data and estimates the flow rate in modeling units (adopted from fd4y.aml, Appendix C7)

```
1: tables
2: select gsfl28.pat
3: unload xxxgsin station_id station_nx m199003 DELIMITED INIT
4: select unprec.pat
5: unload xxxunin unit_id unit_nx gswsh area_km2 order pm199003
   DELIMITED INIT
6: &sys fdy4 xxxgsin xxxunin xxxunout
7: &s i = 0
8: &do &until [exists xxxunout -file]
9:
     &s i = %i% + 1
10:&end
11:define m199003.dat
12:unit id,4,8,B
13:qm199003,4,12,F,4
14:~
15:add from xxxunout
16:select m199003.dat
17:&sys arc joinitem unflow.pat m199003.dat unflow.pat unit_id
   order
18:kill m199003.dat
```



Figure 5.9 Runoff (flow in rivers) that occurred in June 1990 in the Iowa-Cedar River watershed.

5.4.8 Determining input values for the Iowa-Cedar River model

The flow rate at the outlet of each modeling unit has been estimated by the procedure described in Section 5.4.7.

The distributed system of watershed parameters and normal weather parameters have been created for the Iowa-Cedar River using 100 m grid according to the methodology discussed in Section 5.2.2. The concentration models determined by the regression analysis relate agrichemical concentration to parameters of the upstream drainage area. Thus it is important to get parameters for the entire upstream area at each unit watershed outlet rather than data just for the modeling unit belonging to that point. The characteristics of the drainage area that is upstream of each modeling unit outlet, have been extracted from the distributed system of watershed parameters according to the methodology discussed in Section 5.2.5.

5.5 ArcView model of agrichemical transport

The computer version of the agrichemical transport model is completely constructed within the GIS software ArcView. A modular structure has been utilized. Such a structure not only makes the model simple and easy to understand, but also it allows improvement of the model or addition of new blocks without changing the model's core components. The program execution is supported by a customized graphical user interface (GUI). Tools that enhance the graphical representation of the results are developed. The ArcView model contains procedures for representing hydrologic processes.

5.5.1 Model overview

The ArcView application is divided into four projects (a project is a collection of associated documents: views, tables, layouts, charts, and scripts). Each project is designed to perform a different task. Four buttons that allow user to switch between projects have been placed in the PushButton Bar (the avenue scripts assigned to each button are listed in Appendix B1). These buttons have the following functions:

- **a+b** Runs the "model" project. This project is designed to prepare entry data for the agrichemical transport model as well as to calculate concentrations and loads.
- =

Runs the "results" project which is designed to display the results as maps of agrichemical concentration and load.

899 R

Executes project "flwprc" which provides visualization of the flow record for a selected modeling unit.

TLS Project "tools" contains the fundamental tools for hydrologic modeling.

The project "model" is the main component of the ArcView application. Projects "results", "flwprc", and "tools" are supporting modules. The scripts associated with the project "model" are listed in Appendix B2. The scripts used by the projects "results", "flwprc", and "tools" are presented in Appendices B3, B4, and B5, respectively.

The agrichemical transport model is navigated through a set of buttons that, when pressed, execute particular model components. The data entry and the data selection is maintained by a set of windows. Figure 5.10 presents an example of a window that supports selection of the agrichemical application rate to be used for concentration estimation. This window contains three input fields. In the first field, the user can enter the name of agrichemical application database that will be utilized for predicting the chemical concentrations and loads in the Iowa-Cedar River basin. The second field allows user to multiply the application rate in the counties which are selected by ArcView tools. This feature is introduced to study the response of the concentration in rivers after the application rate has been increased or decreased by a specified percentage. The last entry field permits one to specify an application rate for a selected county or all counties without the necessity of editing the attribute tables directly. This field is deactivated if a negative value is entered.

Specify Application Rate	ок
Take values from the database:	2 Cancel
(nonsequence), noting and the second se)[
Multiply data by factor: 1	
Apply specified value: -1	
(negative value deactivates this input field	2.0

Figure 5.10 An example of the Graphical User Interface: a window for the selection of the agrichemical application rate in selected counties.

The presentation tools support drawing bar charts at the center of selected units. They are developed to enhance the presentation of the data and the model results on a map. Figure 5.11 shows examples of the application of the presentation tools.



Figure 5.11 Atrazine concentrations along the Cedar River estimated for 1990 (left) and flow rate along the Cedar River in June 1990 (right).

The hydrologic modeling is supported by scripts that perform the following tasks:

- Selection of the units downstream of a selected point;
- Selection of all units upstream of a selected unit;
- Estimation of the watershed weighted average of an entity such as chemical application rate;
- Accumulation of values when moving downstream (flow accumulation);

- Calculation of the unit mass balance (reverse operation to flow accumulation); and
- Determination of the order of the unit (all exterior units/streams are assigned an order of one, an interior unit has the order equal to the maximum order of the upstream units increased by one).

5.5.2 Project "Model"

When opened, the project "Model" displays the following maps:

- Agrichemical application rate by county (window: Application Rate, theme: Use);
- 2) The Iowa-Cedar River basin divided into modeling units (window: Modeling Units, theme: Units).

Five buttons are designed to select different activities:

Eff Application. This button displays dialog boxes that allow the user to specify the agrichemical application rate. If the view-window "Application Rate" is active, the application in either all, or selected counties can be specified. Additionally, the application rate of nitrogen fertilizers estimated for 1989, 1990, and 1991, and application rate of atrazine estimated for 1989 can be selected. A multiplier that increases/decreases application rate by a given percentage also can be used to simulate the different policy scenarios. If the view-window "Modeling units" is active, the application rate in each modeling unit can be modified.

EQC Edit Cumulative Flow Rate. This button shows dialog boxes for selecting the flow record (by selecting a year) that will be used for calculations and for

adjusting the selected values. For example, all data can be multiplied by a factor that represents extreme conditions. The adjustment may be performed for all months of the specified year or for each individual month.

- Sur Select Year. This button allows the user to specify a year for a model that has a trend component. There is no trend in the current model.
- Select Month. The dialog box displayed by this button specifies if the calculations will be performed for all months or only for selected months of a year.
- Run. Executes the script that performs the calculations.
- First Order Reaction. Calculates concentrations and loads assuming exponential decrease of the agricultural constituent along the flow path. The current model does not contain a map of spatially distributed decay rates that allows one to estimate concentrations by this method.

The following coverages and data files constitute the core database of the model:

1) Coverage cruse--a map of 47 counties that are within the Iowa-Cedar River basin. Table 5.5 presents the items of cruse's PAT.

Field (Item)	Description
Fips	county FIPS code
St	state
Cntyname	county name
N89kgkm2, N90kgkm2	estimated average nitrogen fertilizer application rate for the years
N91kgkm2	1989, 1990, and 1991, respectively [kg/km ²]
A89kgkm2	estimated average atrazine application rate for 1989 [kg/km ²]
Temp	field reserved for storage of results of partial calculations
Use	application rate selected for the estimation of concentrations and
	loads

Table 5.5Polygon Attribute Table of the cruse coverage.

2) Coverage crwsd--map of 1032 modeling units. Table 5.6 lists the items of the attribute table.

Field (Item)	Description
Unit_id	ID of the modeling unit
Gswsh	ID of the USGS gauging station downstream of the modeling unit
Unit_nx	ID of the next unit on the flow path (downstream unit ID)
Order	a number that specifies location of the unit on the flow path
Areakm2	area of the unit [km ²]
Careakm2	drainage area upstream of the unit outlet [km ²]
Alndslp	average land slope of unit drainage area
Alndlgkm	average length on the flow path from the land to the stream network [km]
Chemuse	Agrichemical application rate in the unit [kg/yr/km ²]
Cchemuse	average agrichemical application rate over the unit drainage area
	[kg/yr/km ²]
Travtime	Agrichemical travel time across the unit [d] (no data available)
Losscoef	Overall loss coefficient in the unit [1/d] (no data available)
Expofact	Export factor, fraction of the applied agricultural chemical in the unit
	that enters the surface water (no data available)
Tcavg	Annual average temperature for upstream drainage area [°C]
Pmmavg	Annual precipitation depth, average over upstream drainage area [mm]
Flow01Flow12	monthly flow rate that flows through the unit outlet $[m^3/s]$
Conc01Conc12	concentration at the unit outlet (atrazine [mg/m ³], nitrate plus nitrite as
	nitrogen [g/m ³])
Load01Load12	chemical load (flow * concentration, atrazine [mg/s], nitrate plus nitrite
	as nitrogen [g/s])

Table 5.6Polygon Attribute Table of the crwsd coverage.

3) File Model2a.dbf -- model specification. Table 5.7 shows the fields of this file.

 Table 5.7
 Fields of the file model2a.dbf (model specification).

Field	Description
Year	a year that is used to estimate the trend coefficient;
Ftrend	mathematical description of the trend. Current version of the model assumes no
	trend, i.e. the trend is described by the following equation: 1.00+(0.0000*Year)
Trendcf	trend coefficient which is calculated according to the information stored in
	items Year and Ftrend
Si01Si12	seasonal index, 12 values that represent the monthly variations of the
	agrichemical concentration around the annual average.
Model	model name, e.g. Nitrate01, Atrazine01, Atrazine02
Sel	contains 1 if the model is selected for calculations, 0 otherwise
Equation	equation for estimation of agrichemical concentrations. Four models are
	available,
	1) atrazine model without the flow rate $[\mu g/L]$:
	(-1.5575+(0.026*U)+(0.7998*LL)+(0.4559*TA)-(0.0048*PA))*TR*SI
	2) atrazine model with the flow rate $[\mu g/L]$:
	(-0.8142+(0.0133*U)+(0.3346*LL)+(38.8804*LS)+(0.2732*TA)-
	(0.0029*PA))*(Q^0.2899)*TR*SI
	4) nitrate plus nitrite as nitrogen model without the flow rate [mg/L]:
	(-7.424541+(0.001062*U)-(1.033063*TA)+(0.019339*PA))*TR*SI
	5) nitrate plus nitrite as nitrogen model with the flow rate [mg/L]:
	(-7.57848+(0.00064886*U)+(0.776683*LL)+(173.6409*LS)-
	(0.520245*TA)+(0.0088545*PA))*(Q^0.3432)*TR*SI
	Three multiplicative models are included only for testing purposes:
	x_1 nitrate plus nitrite as nitrogen $[a/m^3]$:
	(0.0001/32008*(1101.381/1)*(0.0.05556))*(0.00.72/0)*(1.1.00.0522)*TP*SI
	x^{2} for atrazine $\left[g/m^{3}\right]$.
	0 0001265546*(UM 8323)*(SLAO 3591)*(OAO 0940)*(LLAO 9208)*TR*SI
	x^3) for atrazine same as (x2) but different output units $[mg/m^3]$
	0.1265546*(U^0.8323)*(SL^0.3591)*(O^0.0940)*(LL^0.9208)*TR*SI
	where: $U = application rate, A = drainage area, Q = flow rate, LL = average$
	overland flow length, $SL = land slope$, $TA = average temperature$, $PA =$
	average precipitation, $TR =$ trend coefficient, and $SI =$ seasonal index.
Comments	comments and model description

- 4) File Linkuse.dbf--description of the link between counties and modeling units (1517 records). Three items describe the link: Fips (county FIPS code), Unit_id (ID number of the modeling unit or part of the modeling unit that is located in the county described by the FIPS code), and Area_km2 (area of the unit or part of the unit that is located in the county specified by the FIPS code [km²]).
- 5) Coverage Unflow -- map of 1032 modeling units. The PAT file contains item Unit_id, and items Qm196001...Qm199209, that store the cumulative flow rate estimated for the period from January 1960 to September 1992.
- 6) Coverage Unprec -- map of 1033 modeling units. The PAT file contains item Unit_id, and items Pm195001...Pm199306, that store the average precipitation depth estimated for the period from January 1950 to June 1993.

The ArcView script equat6 (Appendix B2) calculates concentrations and loads. This script first selects the record that contains the value of item [Sel] equal to 1. Then equat6 extracts the value from the item [Year], retrieves the equation that describes the trend from the item [Ftrend], calculates the trend coefficient, and stores it in the item [Trendcf].

In the next step, the script extracts the equation from the item [Equation] and replaces the symbolic names U, A, LS, LL, and Q with the corresponding item names [Cchemuse], [Careakm2], [Alndslp], [Alndlgkm], and one of the item [Qm01]...[Qm12]. The symbolic name TR is replaced by the value stored in the item [Trendcf] and the name SI is replaced by the value from one of the items [Si01]...[Si12]. The concentrations are calculated for each month of the year by the Avenue request calculate and the results are stored in the items

[Conc01]..[Conc12]. The loads are estimated by multiplication of the flows and concentrations. The products are stored in the items [Load01]...[Load12].

Calculations of the agrichemical concentration in surface waters, according to the first order process, are performed by the script decay1. This Avenue program has been written for future extentions of the agrichemical transport model, for example, to utilize the results of the CEEPES (Comprehensive Environmental Economic Policy Evaluation System) modeling program developed by Iowa State University's Center for Agricultural and Rural Development, CARD (Bouzaher and Monale, 1993).

5.5.3 Project "Results"

This project reserves the space for preparing the maps of estimated agrichemical concentration and load in surface water. Three scripts, executed from the button bar, \blacksquare , \blacksquare , and \blacksquare , draw the bar charts of the monthly average chemical concentration, chemical load and flow rate, respectively. Figure 5.13 presents the preliminary agrichemical model results of the estimation atrazine concentrations in 1990 in the form of bar charts located along the Iowa River and the Cedar River.



Figure 5.12 "Bar chart" map of the atrazine concentrations estimated for 1990 (preliminary results)-- an example map created within the ArcView project "Results" (g/m3 = mg/L).

The results of the calculations can be presented on the map of modeling units. Figure 5.13 shows an example of atrazine concentrations in streams for May 1990.



Figure 5.13 Atrazine concentrations in the Cedar River basin introductory estimated for May 1990 -- a map created within the ArcView project "Results" (g/m3 = mg/L).

The ArcView model of the agrichemical transport represents the flow system as a network of connected modeling units. Since the Arc/Info-Grid procedures that

convert grid of rivers into vector format do not preserve proper numbering of the stream reaches, i.e., some reaches are split and they are identified by two or more IDs (Fig. 5.14), the modeling unit approach has been used to simplify the model.



Figure 5.14 Inconsistency in the assigning IDs to the vectorized grid streams. The GRID function gridline assigned wrong IDs to the Cedar River downstream to the junction with the Iowa River.

The vector representation of the stream network created by both, streamline and gridline commands can not be used for the modeling without extensive editing of the stream coverage. However, such a map of rivers can be used for data presentation purposes. Figure 5.15 shows flow rate in the streams of the Iowa-Cedar Basin created by linking the polygon attribute table of modeling unit coverage with the arc attribute table of the streams map.



Figure 5.15 Flow rate in the Cedar River and tributaries that occurred in June 1990. The map has been created by linking the polygon attribute table of interpolated flow measurements by modeling unit with the arc attribute table of a stream coverage.

5.5.4 Project "Flwprc"

The bar charts that represent the monthly flow rate and the average precipitation depth for a selected time period can be drawn at the center of selected modeling units (i draws charts of the flow rate and i draws charts of the precipitation depth). The script associated with the button i displays all recorded flow rate (monthly values from January 1960 to December 1992) for a specified modeling unit. Since charts of monthly flow rate for multiple year periods can be drawn, the wet or dry years can be easily identified. Figure 5.16 presents the monthly flow for years from 1989 to 1991.



Figure 5.16 Monthly flow rate in the lower Cedar River in 1989-1991. Example of visual tools of ArcView project "Flwprc" for hydrologic analysis.

5.5.5 Project "Tools"

The following tools have been created to support the model of agrichemicals in surface waters (Avenue scripts are included in Appendix B5):

- Determines the unit/stream order in the flow system (Avenue script order6);
- Calculates weighted average for each modeling unit total drainage area (script upavg2);
- **E** Accumulates values going along the flow path (script cumul2); and
- Calculates the difference between the unit inputs and the unit output (script decom2).