

TABLEAU 4 : Optima et tolérances estimées des espèces

TABLE 4: Optima and tolerances of the species

Weighted Averaging (WA) method. Results: R, R<sup>2</sup>, Standard error of prediction (SEP).  
Weighted Averaging Plus Least Squares regression (WA-PLS). Results: number of components, r, R, R<sup>2</sup> and S

| Genres       | Espèces                     | Codes   | Na+ (mg/l) |          |           |           |
|--------------|-----------------------------|---------|------------|----------|-----------|-----------|
| Genera       | Species                     | Samples | codes      | OPTIMUM  | TOLERANCE | FREQUENCE |
| Achnanthes   | arenaria                    | ACAR    |            | 9440.02  | 11850.67  | 6         |
| Achnanthes   | delicatula                  | AD      |            | 13217.75 | 17837.34  | 7         |
| Achnanthes   | speciosa                    | ASPE    |            | 9437.31  | 4670.60   | 6         |
| Amphora      | atacamana                   | AMPA    |            | 40443.13 | 32684.07  | 17        |
| Amphora      | atacamana minor             | AMPM    |            | 40196.09 | 36663.85  | 7         |
| Amphora      | boliviana                   | ABOL    |            | 23994.03 | 17053.50  | 5         |
| Amphora      | boliviana elongata          | ABEL    |            | 10787.01 | 25830.84  | 9         |
| Amphora      | carvajaliana                | AMCJ    |            | 15297.68 | 11510.65  | 21        |
| Anomooneis   | sphaerophora angusta        | ANSA    |            | 13427.04 | 10983.83  | 9         |
| Caloneis     | silicula minuta             | CSP     |            | 16067.21 | 14089.92  | 4         |
| Caloneis     | westii                      | CAW     |            | 3332.06  | 9349.22   | 8         |
| Cocconeis    | placentula                  | CP      |            | 7358.88  | 6013.96   | 7         |
| Cymbella     | gracilis                    | CYL     |            | 9520.02  | 10816.22  | 13        |
| Cymbella     | pusilla                     | CYMP    |            | 21344.87 | 15054.82  | 7         |
| Denticula    | thermalis                   | DETH    |            | 6761.96  | 4415.52   | 5         |
| Fragilaria   | brevistriata                | FB      |            | 17235.64 | 33302.23  | 11        |
| Fragilaria   | construens venter           | FRCV    |            | 26823.29 | 29188.60  | 5         |
| Fragilaria   | fasciculata                 | FE      |            | 37721.56 | 34753.68  | 5         |
| Fragilaria   | leptaustoron martyi         | OM      |            | 27283.28 | 29857.10  | 7         |
| Fragilaria   | pinnata                     | FP      |            | 37365.34 | 41497.84  | 9         |
| Fragilaria   | zeilleri                    | FZ      |            | 177.13   | 488.35    | 4         |
| Hantzschia   | amphioxys                   | HA      |            | 27347.08 | 38222.20  | 4         |
| Hantzschia   | nov. sp.                    | HN      |            | 2085.29  | 10485.98  | 7         |
| Mastoglia    | atacamae                    | MATA    |            | 6873.58  | 15864.44  | 11        |
| Navicula     | cariocincta                 | NCA     |            | 22097.43 | 34459.92  | 14        |
| Navicula     | cincta                      | NCI     |            | 50355.07 | 38808.34  | 4         |
| Navicula     | veneta                      | NC      |            | 9779.83  | 20579.58  | 20        |
| Navicula     | nivalis                     | NHN     |            | 4366.02  | 18936.03  | 5         |
| Navicula     | paramutica binodis          | NPB     |            | 6935.49  | 19702.86  | 9         |
| Navicula     | cryptotenelloides           | NAO     |            | 28421.04 | 34981.70  | 25        |
| Navicula     | pseudolanceolata            | NLA     |            | 16821.11 | 12651.41  | 7         |
| Navicula     | pseudolitoricola            | NLI     |            | 12031.41 | 14350.63  | 5         |
| Fallacia     | pygmae                      | NPYG    |            | 3339.75  | 4620.82   | 7         |
| Navicula     | erifuga                     | NDC     |            | 28247.65 | 28971.50  | 19        |
| Navicula     | salinicola                  | NASA    |            | 55122.24 | 34786.00  | 18        |
| Navicula     | sp.                         | NS      |            | 13124.38 | 30099.34  | 5         |
| Nitzschia    | liebetruthii                | NILI    |            | 8307.35  | 3635.29   | 6         |
| Nitzschia    | accedens chilensis          | NCHI    |            | 48925.66 | 38497.14  | 17        |
| Nitzschia    | alpina                      | NIAL    |            | 25431.24 | 19047.58  | 7         |
| Nitzschia    | amphibiodes                 | ND      |            | 8500.04  | 7345.89   | 4         |
| Nitzschia    | compressa compressa         | NICC    |            | 14086.18 | 24500.73  | 13        |
| Nitzschia    | epithemioides epithemioides | NIEP    |            | 52051.10 | 37543.32  | 12        |
| Nitzschia    | frustulum                   | NF      |            | 13205.34 | 20836.79  | 16        |
| Nitzschia    | grunowii                    | NGRU    |            | 9150.83  | 5819.79   | 8         |
| Nitzschia    | hantzschiana                | NIH     |            | 6869.44  | 10104.02  | 12        |
| Nitzschia    | hungarica                   | NIHU    |            | 9519.94  | 17046.45  | 20        |
| Nitzschia    | palea                       | NPA     |            | 64909.73 | 28127.99  | 6         |
| Nitzschia    | pusilla                     | NIPS    |            | 69579.49 | 35585.78  | 11        |
| Nitzschia    | valdecostata                | NIVA    |            | 5422.61  | 4662.80   | 7         |
| Pinnularia   | bogotensis                  | PB      |            | 8636.53  | 17258.04  | 6         |
| Pinnularia   | microstauron                | PIMI    |            | 6689.21  | 22072.75  | 5         |
| Rhopalodia   | wetzelii                    | RHWE    |            | 24527.57 | 27391.25  | 14        |
| Scoliopleura | peisonis                    | SCPE    |            | 14800.99 | 13101.88  | 13        |
| Stauroneis   | gregorii                    | SG      |            | 26378.85 | 30284.68  | 13        |
| Stauroneis   | bathurstensis               | SB      |            | 10397.72 | 6982.38   | 7         |
| Stauroneis   | species (obtus?)            | SSP     |            | 10391.23 | 1275.46   | 4         |
| Stauroneis   | wislouchii                  | STAW    |            | 21298.95 | 18691.32  | 13        |
| Surirella    | oregonica                   | SO      |            | 18356.95 | 35103.41  | 4         |
| Surirella    | sella                       | SUSE    |            | 7995.52  | 9242.72   | 19        |
| Surirella    | sp.                         | SUSP    |            | 4010.54  | 1994.34   | 6         |
| Surirella    | wetzelii                    | SUWE    |            | 19125.02 | 14219.46  | 21        |

| <i>Samples</i>                                                   | <i>Observed values</i> | <i>Estimated values</i> | <i>Residus</i>              |
|------------------------------------------------------------------|------------------------|-------------------------|-----------------------------|
| BA67                                                             | 13600.000              | 9850.410                | 3749.590                    |
| RAM6                                                             | 7590.000               | 9189.363                | -1599.363                   |
| VER5                                                             | 4510.000               | 10314.528               | -5804.528                   |
| HED4                                                             | 20400.000              | 15766.853               | 4633.147                    |
| PJ30                                                             | 10000.000              | 17438.639               | -7438.639                   |
| PUR2                                                             | 9550.000               | 17764.068               | -8214.068                   |
| HON4                                                             | 6740.000               | 15732.725               | -8992.725                   |
| CHI5                                                             | 20700.000              | 16570.824               | 4129.176                    |
| CAN4                                                             | 3590.000               | 17847.662               | -14257.662                  |
| CHU4                                                             | 30100.000              | 16336.339               | 13763.661                   |
| CHU9                                                             | 2320.000               | 15377.588               | -13057.588                  |
| CL20                                                             | 10600.000              | 21038.520               | -10438.520                  |
| CD24                                                             | 19900.000              | 22094.158               | -2194.158                   |
| CD16                                                             | 40700.000              | 31594.473               | 9105.527                    |
| PG70                                                             | 4000.000               | 17107.711               | -13107.711                  |
| PG23                                                             | 451.000                | 15642.589               | -15191.589                  |
| PG41                                                             | 9270.000               | 33827.559               | -24557.559                  |
| PG43                                                             | 4510.000               | 37911.148               | -33401.148                  |
| PG45                                                             | 34000.000              | 36413.168               | -2413.168                   |
| PG47                                                             | 103000.000             | 43389.824               | 59610.176                   |
| PG72                                                             | 80.000                 | 8339.988                | -8259.988                   |
| PG73                                                             | 3910.000               | 12262.317               | -8352.317                   |
| PG76                                                             | 4510.000               | 19992.775               | -15482.775                  |
| PG74                                                             | 350.000                | 11090.177               | -10740.177                  |
| PG78                                                             | 46000.000              | 31939.594               | 14060.406                   |
| PG82                                                             | 41.900                 | 15822.397               | -15780.497                  |
| PG84                                                             | 77100.000              | 47132.605               | 29967.395                   |
| PG97                                                             | 85.100                 | 16681.498               | -16596.398                  |
| P114                                                             | 81000.000              | 41826.746               | 39173.254                   |
| P116                                                             | 92000.000              | 43336.016               | 48663.984                   |
| <i>WA: Coefficient de corrélation multiple</i>                   |                        |                         | <b>R = 0.8117</b>           |
|                                                                  |                        |                         | <b>R<sup>2</sup> = 0.66</b> |
| <i>Variance de la variable Na à expliquer</i>                    |                        |                         | <b>8.31E+08</b>             |
| <i>Variance des résidus</i>                                      |                        |                         | <b>4.25E+08</b>             |
| <i>Ecart-type des résidus = SEP Standard error of prediction</i> |                        |                         | <b>20614.64</b>             |
| <i>WA-PLS : 2 components, SEP = 19442</i>                        |                        |                         | <b>R = 0.89</b>             |
|                                                                  |                        |                         | <b>R<sup>2</sup> = 0.80</b> |
|                                                                  |                        |                         | <b>r = 0.7428</b>           |

| K+ (mg/l)    |                |                  |                  | Salinity (mg/l) |                |                  |                  |
|--------------|----------------|------------------|------------------|-----------------|----------------|------------------|------------------|
| <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i>    | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|              | 1207.12        | 925.77           | 6                |                 | 29884.19       | 34429.63         | 6                |
|              | 1511.25        | 2143.75          | 7                |                 | 40795.95       | 55567.99         | 7                |
|              | 1166.47        | 600.42           | 6                |                 | 31176.80       | 15906.11         | 6                |
|              | 4426.33        | 3845.48          | 17               |                 | 123735.41      | 99822.04         | 17               |
|              | 4257.09        | 4103.14          | 7                |                 | 122779.11      | 110397.41        | 7                |
|              | 2860.24        | 1447.47          | 5                |                 | 72972.30       | 48567.10         | 5                |
|              | 1825.20        | 3406.29          | 9                |                 | 34962.11       | 80398.52         | 9                |
|              | 2077.72        | 2147.55          | 21               |                 | 50363.23       | 37055.72         | 21               |
|              | 2897.28        | 3823.70          | 9                |                 | 44776.31       | 38354.55         | 9                |
|              | 6951.01        | 5887.35          | 4                |                 | 64038.06       | 55436.06         | 4                |
|              | 350.89         | 795.83           | 8                |                 | 10419.22       | 27379.88         | 8                |
|              | 923.81         | 743.64           | 7                |                 | 23819.22       | 17230.23         | 7                |
|              | 1071.23        | 1196.17          | 13               |                 | 30254.42       | 33905.07         | 13               |
|              | 4631.94        | 4764.32          | 7                |                 | 71689.87       | 48995.69         | 7                |
|              | 1464.69        | 419.25           | 5                |                 | 24453.56       | 13426.39         | 5                |
|              | 2142.83        | 4228.09          | 11               |                 | 53828.97       | 103370.23        | 11               |
|              | 2866.36        | 3155.15          | 5                |                 | 82480.13       | 89476.72         | 5                |
|              | 4810.78        | 4884.37          | 5                |                 | 116897.13      | 109656.84        | 5                |
|              | 2635.38        | 2740.90          | 7                |                 | 81122.17       | 88503.35         | 7                |
|              | 3477.70        | 3933.59          | 9                |                 | 110897.58      | 122287.35        | 9                |
|              | 18.46          | 53.66            | 4                |                 | 627.79         | 1512.63          | 4                |
|              | 3312.03        | 4629.13          | 4                |                 | 86242.18       | 120386.45        | 4                |
|              | 288.91         | 1278.51          | 7                |                 | 6799.33        | 32799.58         | 7                |
|              | 705.25         | 1446.05          | 11               |                 | 21127.10       | 46977.82         | 11               |
|              | 2131.09        | 3435.69          | 14               |                 | 66718.63       | 103268.48        | 14               |
|              | 5849.73        | 4612.14          | 4                |                 | 157232.81      | 121336.81        | 4                |
|              | 1264.47        | 2378.74          | 20               |                 | 30542.75       | 62613.84         | 20               |
|              | 369.78         | 1523.23          | 5                |                 | 12920.90       | 54997.88         | 5                |
|              | 1541.78        | 3682.57          | 9                |                 | 23503.87       | 61560.73         | 9                |
|              | 3238.18        | 4138.50          | 25               |                 | 87662.23       | 107368.46        | 25               |
|              | 6070.26        | 5953.59          | 7                |                 | 63646.28       | 50895.54         | 7                |
|              | 1407.68        | 1534.89          | 5                |                 | 38474.49       | 44953.49         | 5                |
|              | 400.11         | 569.66           | 7                |                 | 10917.80       | 15497.66         | 7                |
|              | 3065.24        | 3031.91          | 19               |                 | 86752.94       | 87606.20         | 19               |
|              | 5914.08        | 4163.34          | 18               |                 | 167355.16      | 106348.25        | 18               |
|              | 1732.16        | 4169.37          | 5                |                 | 41231.30       | 94724.01         | 5                |
|              | 983.03         | 547.96           | 6                |                 | 28432.38       | 12116.65         | 6                |
|              | 5219.24        | 4429.53          | 17               |                 | 148070.84      | 116343.82        | 17               |
|              | 2867.35        | 2681.80          | 7                |                 | 76748.71       | 59978.92         | 7                |
|              | 856.53         | 866.66           | 4                |                 | 26391.02       | 22403.08         | 4                |
|              | 1313.88        | 2022.91          | 13               |                 | 42439.33       | 71431.60         | 13               |
|              | 5416.01        | 4283.07          | 12               |                 | 157145.11      | 113644.09        | 12               |
|              | 2049.83        | 3191.30          | 16               |                 | 42566.63       | 64692.72         | 16               |
|              | 1249.43        | 614.71           | 8                |                 | 29977.37       | 17128.71         | 8                |
|              | 1199.49        | 2455.08          | 12               |                 | 23025.32       | 33768.41         | 12               |
|              | 2176.01        | 3286.98          | 20               |                 | 32533.97       | 53575.68         | 20               |
|              | 5508.15        | 2199.18          | 6                |                 | 190057.30      | 81420.38         | 6                |
|              | 7761.39        | 4335.74          | 11               |                 | 212075.11      | 108571.73        | 11               |
|              | 586.82         | 652.96           | 7                |                 | 17276.65       | 14251.57         | 7                |
|              | 2315.01        | 4612.97          | 6                |                 | 30407.47       | 57011.78         | 6                |
|              | 1085.02        | 1823.82          | 5                |                 | 21220.58       | 63804.37         | 5                |
|              | 2710.03        | 3007.51          | 14               |                 | 74965.75       | 82850.99         | 14               |
|              | 1708.77        | 1435.23          | 13               |                 | 47373.04       | 40977.83         | 13               |
|              | 3107.44        | 3915.96          | 13               |                 | 82300.65       | 94715.86         | 13               |
|              | 1148.16        | 801.92           | 7                |                 | 33961.54       | 23164.52         | 7                |
|              | 2769.21        | 435.99           | 4                |                 | 35521.27       | 4497.50          | 4                |
|              | 3094.82        | 1616.26          | 13               |                 | 65771.20       | 53788.02         | 13               |
|              | 2472.09        | 4863.69          | 4                |                 | 57857.84       | 110435.44        | 4                |
|              | 972.41         | 1242.84          | 19               |                 | 25807.73       | 28999.84         | 19               |
|              | 461.16         | 249.10           | 6                |                 | 12834.27       | 6515.62          | 6                |
|              | 5394.96        | 5449.09          | 21               |                 | 69143.63       | 51302.73         | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 1700.000                                                         | 1190.587                | 509.413                     | 45335.000                                                        | 32671.533               | 12663.467                   |
| 1030.000                                                         | 1100.207                | -70.207                     | 27658.000                                                        | 30878.086               | -3220.086                   |
| 308.000                                                          | 1204.500                | -896.500                    | 14716.000                                                        | 34239.449               | -19523.449                  |
| 2100.000                                                         | 2508.819                | -408.819                    | 67099.000                                                        | 52600.191               | 14498.809                   |
| 1020.000                                                         | 2161.026                | -1141.026                   | 31139.000                                                        | 55710.945               | -24571.945                  |
| 1720.000                                                         | 2335.447                | -615.447                    | 32785.000                                                        | 57165.410               | -24380.410                  |
| 989.000                                                          | 2062.277                | -1073.277                   | 21392.000                                                        | 50968.250               | -29576.250                  |
| 2500.000                                                         | 2163.798                | 336.202                     | 69439.000                                                        | 53829.586               | 15609.414                   |
| 212.000                                                          | 3499.940                | -3287.940                   | 11440.000                                                        | 59072.313               | -47632.313                  |
| 12800.000                                                        | 4922.541                | 7877.459                    | 119261.000                                                       | 59508.641               | 59752.359                   |
| 1800.000                                                         | 2976.847                | -1176.847                   | 11377.000                                                        | 50853.691               | -39476.691                  |
| 2850.000                                                         | 3194.134                | -344.134                    | 36285.000                                                        | 65473.848               | -29188.848                  |
| 2110.000                                                         | 3085.000                | -975.000                    | 59166.000                                                        | 68947.984               | -9781.984                   |
| 4260.000                                                         | 3810.768                | 449.232                     | 120357.000                                                       | 96830.477               | 23526.523                   |
| 532.000                                                          | 2218.201                | -1686.201                   | 12787.000                                                        | 54032.887               | -41245.887                  |
| 43.000                                                           | 1913.913                | -1870.913                   | 1475.000                                                         | 48721.523               | -47246.523                  |
| 1020.000                                                         | 3764.239                | -2744.239                   | 28564.000                                                        | 103717.336              | -75153.336                  |
| 500.000                                                          | 4202.771                | -3702.771                   | 13961.000                                                        | 115942.891              | -101981.891                 |
| 3950.000                                                         | 4206.625                | -256.625                    | 103267.000                                                       | 111875.195              | -8608.195                   |
| 14200.000                                                        | 4819.732                | 9380.268                    | 324141.000                                                       | 132470.984              | 191670.016                  |
| 16.500                                                           | 1244.068                | -1227.568                   | 644.000                                                          | 26697.957               | -26053.957                  |
| 399.000                                                          | 2304.313                | -1905.313                   | 12189.000                                                        | 40753.777               | -28564.777                  |
| 579.000                                                          | 2433.364                | -1854.364                   | 14421.000                                                        | 62155.457               | -47734.457                  |
| 48.100                                                           | 1482.448                | -1434.349                   | 1542.000                                                         | 35173.887               | -33631.887                  |
| 5000.000                                                         | 3514.777                | 1485.223                    | 144099.000                                                       | 97949.422               | 46149.578                   |
| 4.420                                                            | 1703.133                | -1698.713                   | 195.000                                                          | 48293.891               | -48098.891                  |
| 6450.000                                                         | 5043.687                | 1406.313                    | 225344.000                                                       | 142971.688              | 82372.313                   |
| 12.600                                                           | 2056.703                | -2044.103                   | 402.000                                                          | 51884.598               | -51482.598                  |
| 9810.000                                                         | 4639.320                | 5170.680                    | 255230.000                                                       | 127894.984              | 127335.016                  |
| 7390.000                                                         | 4677.638                | 2712.362                    | 267366.000                                                       | 131722.109              | 135643.891                  |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.7559</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.8022</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.57</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.57</b> |
| <b>Variance de la variable K à expliquer</b>                     |                         | <b>1.37E+07</b>             | <b>Variance de la variable Salinité à expliquer</b>              |                         | <b>7.69E+09</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>8377185</b>              | <b>Variance des résidus</b>                                      |                         | <b>4.07E+09</b>             |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>2894.337</b>             | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>63814.21</b>             |
| <b>WA-PLS : 1 component</b>                                      |                         |                             | <b>WA-PLS : 2 components, SEP = 62130</b>                        |                         | <b>R = 0.8849</b>           |
|                                                                  |                         |                             |                                                                  |                         | <b>R<sup>2</sup> = 0.78</b> |
|                                                                  |                         |                             |                                                                  |                         | <b>r = 0.71</b>             |

| Alkalinity meq/l |                |                  |                  | Mg++ (mg/l)  |                |                  |                  |
|------------------|----------------|------------------|------------------|--------------|----------------|------------------|------------------|
| <i>codes</i>     | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|                  | 4.83           | 2.42             | 6                |              | 255.58         | 302.83           | 6                |
|                  | 4.96           | 3.53             | 7                |              | 259.71         | 498.06           | 7                |
|                  | 4.81           | 0.48             | 6                |              | 393.67         | 236.63           | 6                |
|                  | 9.55           | 6.85             | 17               |              | 934.53         | 1001.13          | 17               |
|                  | 8.77           | 5.79             | 7                |              | 1114.11        | 1031.01          | 7                |
|                  | 19.57          | 12.10            | 5                |              | 609.18         | 351.06           | 5                |
|                  | 7.83           | 5.10             | 9                |              | 310.19         | 837.84           | 9                |
|                  | 8.45           | 5.60             | 21               |              | 559.31         | 507.79           | 21               |
|                  | 12.83          | 9.73             | 9                |              | 436.95         | 583.08           | 9                |
|                  | 21.54          | 13.74            | 4                |              | 976.78         | 925.04           | 4                |
|                  | 4.00           | 1.65             | 8                |              | 96.89          | 159.22           | 8                |
|                  | 7.93           | 3.34             | 7                |              | 251.37         | 105.36           | 7                |
|                  | 5.76           | 2.04             | 13               |              | 279.62         | 315.07           | 13               |
|                  | 18.34          | 14.90            | 7                |              | 811.12         | 681.13           | 7                |
|                  | 7.05           | 3.65             | 5                |              | 267.74         | 218.89           | 5                |
|                  | 5.14           | 6.02             | 11               |              | 526.02         | 1045.61          | 11               |
|                  | 5.67           | 2.19             | 5                |              | 699.55         | 774.64           | 5                |
|                  | 9.92           | 6.88             | 5                |              | 787.64         | 1328.67          | 5                |
|                  | 8.16           | 5.01             | 7                |              | 515.12         | 666.24           | 7                |
|                  | 6.86           | 6.51             | 9                |              | 848.94         | 1063.83          | 9                |
|                  | 0.85           | 0.76             | 4                |              | 7.73           | 16.18            | 4                |
|                  | 3.37           | 3.08             | 4                |              | 863.02         | 1201.80          | 4                |
|                  | 3.02           | 2.67             | 7                |              | 67.10          | 316.65           | 7                |
|                  | 4.85           | 1.77             | 11               |              | 170.92         | 316.38           | 11               |
|                  | 3.82           | 4.47             | 14               |              | 519.20         | 852.05           | 14               |
|                  | 5.22           | 3.57             | 4                |              | 1485.00        | 1200.18          | 4                |
|                  | 6.80           | 5.04             | 20               |              | 261.44         | 571.33           | 20               |
|                  | 2.24           | 2.49             | 5                |              | 105.26         | 426.55           | 5                |
|                  | 6.04           | 8.87             | 9                |              | 260.79         | 643.18           | 9                |
|                  | 7.45           | 7.39             | 25               |              | 759.29         | 1050.31          | 25               |
|                  | 18.84          | 14.61            | 7                |              | 901.39         | 884.16           | 7                |
|                  | 4.86           | 2.03             | 5                |              | 375.59         | 403.90           | 5                |
|                  | 2.69           | 1.74             | 7                |              | 126.12         | 239.36           | 7                |
|                  | 7.77           | 5.70             | 19               |              | 662.75         | 805.69           | 19               |
|                  | 12.08          | 8.31             | 18               |              | 1351.85        | 1118.83          | 18               |
|                  | 4.95           | 6.07             | 5                |              | 434.87         | 1015.02          | 5                |
|                  | 4.95           | 1.81             | 6                |              | 382.49         | 145.35           | 6                |
|                  | 26.48          | 68.77            | 17               |              | 1251.83        | 1133.28          | 17               |
|                  | 14.67          | 6.52             | 7                |              | 592.65         | 676.83           | 7                |
|                  | 5.26           | 4.32             | 4                |              | 203.84         | 283.87           | 4                |
|                  | 5.70           | 2.34             | 13               |              | 325.96         | 480.09           | 13               |
|                  | 9.98           | 7.00             | 12               |              | 1212.33        | 1150.28          | 12               |
|                  | 6.96           | 6.71             | 16               |              | 376.29         | 624.60           | 16               |
|                  | 7.45           | 4.09             | 8                |              | 274.68         | 214.97           | 8                |
|                  | 6.25           | 6.17             | 12               |              | 235.63         | 394.34           | 12               |
|                  | 9.22           | 8.70             | 20               |              | 287.81         | 596.76           | 20               |
|                  | 21.86          | 66.12            | 6                |              | 1081.25        | 490.77           | 6                |
|                  | 24.73          | 62.45            | 11               |              | 1840.32        | 1214.60          | 11               |
|                  | 4.14           | 3.21             | 7                |              | 101.32         | 112.42           | 7                |
|                  | 8.67           | 11.32            | 6                |              | 392.05         | 680.48           | 6                |
|                  | 6.50           | 4.37             | 5                |              | 171.03         | 493.83           | 5                |
|                  | 6.55           | 3.88             | 14               |              | 451.37         | 747.87           | 14               |
|                  | 6.41           | 2.45             | 13               |              | 427.65         | 422.44           | 13               |
|                  | 7.24           | 5.49             | 13               |              | 703.45         | 958.14           | 13               |
|                  | 6.11           | 3.14             | 7                |              | 293.92         | 281.30           | 7                |
|                  | 343.05         | 63.68            | 4                |              | 4.85           | 30.72            | 4                |
|                  | 190.15         | 167.55           | 13               |              | 353.31         | 500.26           | 13               |
|                  | 6.71           | 6.78             | 4                |              | 609.79         | 1186.10          | 4                |
|                  | 5.62           | 3.01             | 19               |              | 253.96         | 304.65           | 19               |
|                  | 4.34           | 0.92             | 6                |              | 137.36         | 63.04            | 6                |
|                  | 16.68          | 13.32            | 21               |              | 854.15         | 817.65           | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 4.880                                                            | 5.629                   | -0.749                      | 605.000                                                          | 386.463                 | 218.537                     |
| 2.930                                                            | 5.367                   | -2.437                      | 326.000                                                          | 385.820                 | -59.820                     |
| 7.250                                                            | 5.943                   | 1.307                       | 262.000                                                          | 416.459                 | -154.459                    |
| 10.000                                                           | 9.825                   | 0.175                       | 649.000                                                          | 585.043                 | 63.957                      |
| 7.220                                                            | 7.909                   | -0.689                      | 210.000                                                          | 542.507                 | -332.507                    |
| 7.800                                                            | 8.281                   | -0.481                      | 275.000                                                          | 568.564                 | -293.564                    |
| 4.400                                                            | 7.968                   | -3.568                      | 140.000                                                          | 525.182                 | -385.182                    |
| 8.050                                                            | 9.280                   | -1.230                      | 1140.000                                                         | 570.364                 | 569.636                     |
| 2.150                                                            | 33.674                  | -31.524                     | 34.000                                                           | 577.680                 | -543.680                    |
| 35.000                                                           | 17.005                  | 17.995                      | 1900.000                                                         | 772.366                 | 1127.634                    |
| 11.400                                                           | 11.218                  | 0.182                       | 53.000                                                           | 506.815                 | -453.815                    |
| 355.000                                                          | 211.978                 | 143.022                     | 0.146                                                            | 342.099                 | -341.953                    |
| 12.900                                                           | 21.075                  | -8.175                      | 382.000                                                          | 593.984                 | -211.984                    |
| 31.500                                                           | 85.025                  | -53.525                     | 914.000                                                          | 721.933                 | 192.067                     |
| 5.090                                                            | 6.856                   | -1.766                      | 89.900                                                           | 506.458                 | -416.558                    |
| 1.510                                                            | 5.726                   | -4.216                      | 11.000                                                           | 459.126                 | -448.126                    |
| 4.250                                                            | 15.215                  | -10.965                     | 265.000                                                          | 856.742                 | -591.742                    |
| 3.210                                                            | 10.760                  | -7.550                      | 132.000                                                          | 933.127                 | -801.127                    |
| 9.080                                                            | 10.065                  | -0.985                      | 110.000                                                          | 883.374                 | -773.374                    |
| 22.900                                                           | 12.948                  | 9.952                       | 3470.000                                                         | 1097.798                | 2372.202                    |
| 3.300                                                            | 6.202                   | -2.902                      | 20.200                                                           | 246.155                 | -225.955                    |
| 5.130                                                            | 9.467                   | -4.337                      | 138.000                                                          | 427.681                 | -289.681                    |
| 3.850                                                            | 17.223                  | -13.373                     | 132.000                                                          | 497.498                 | -365.498                    |
| 4.200                                                            | 6.356                   | -2.156                      | 55.400                                                           | 320.698                 | -265.298                    |
| 9.420                                                            | 8.664                   | 0.756                       | 1200.000                                                         | 793.382                 | 406.618                     |
| 0.523                                                            | 4.055                   | -3.532                      | 3.210                                                            | 398.847                 | -395.637                    |
| 9.700                                                            | 20.107                  | -10.407                     | 1250.000                                                         | 1129.245                | 120.755                     |
| 1.360                                                            | 7.315                   | -5.955                      | 7.410                                                            | 446.102                 | -438.692                    |
| 7.680                                                            | 12.414                  | -4.734                      | 2550.000                                                         | 1071.368                | 1478.632                    |
| 13.100                                                           | 15.249                  | -2.149                      | 2080.000                                                         | 1080.861                | 999.139                     |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.9460</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.7260</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.89</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.53</b> |
| <b>Variance de la variable Alcalinité à expliquer</b>            |                         | <b>3929.396</b>             | <b>Variance de la variable Mg à expliquer</b>                    |                         | <b>724201.7</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>847.3527</b>             | <b>Variance des résidus</b>                                      |                         | <b>478831.7</b>             |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>29.10932</b>             | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>691.9767</b>             |
| <b>WA-PLS : 2 components, SEP = 62.26</b>                        |                         | <b>R = 0.9661</b>           | <b>WA-PLS : 2 components, SEP = 857</b>                          |                         | <b>R = 0.8437</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.93</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.71</b> |
|                                                                  |                         | <b>r = 0.29</b>             |                                                                  |                         | <b>r = 0.43</b>             |

| Ca++ (mg/l)  |                |                  |                  | pH           |                |                  |                  |
|--------------|----------------|------------------|------------------|--------------|----------------|------------------|------------------|
| <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|              | 420.70         | 482.06           | 6                |              | 8.86           | 0.38             | 6                |
|              | 450.58         | 515.59           | 7                |              | 8.20           | 0.59             | 7                |
|              | 768.25         | 499.24           | 6                |              | 8.22           | 0.10             | 6                |
|              | 1137.33        | 899.67           | 17               |              | 7.93           | 0.60             | 17               |
|              | 1267.27        | 1008.59          | 7                |              | 7.98           | 0.42             | 7                |
|              | 425.29         | 380.82           | 5                |              | 8.75           | 0.73             | 5                |
|              | 391.49         | 746.98           | 9                |              | 8.70           | 1.04             | 9                |
|              | 618.80         | 470.62           | 21               |              | 8.57           | 0.34             | 21               |
|              | 224.58         | 217.28           | 9                |              | 8.92           | 0.63             | 9                |
|              | 444.63         | 289.77           | 4                |              | 8.89           | 1.01             | 4                |
|              | 149.26         | 253.17           | 8                |              | 8.42           | 0.59             | 8                |
|              | 347.14         | 401.19           | 7                |              | 8.84           | 0.58             | 7                |
|              | 452.72         | 458.50           | 13               |              | 8.34           | 0.42             | 13               |
|              | 559.39         | 447.41           | 7                |              | 8.67           | 0.41             | 7                |
|              | 724.62         | 544.64           | 5                |              | 9.07           | 0.95             | 5                |
|              | 533.64         | 965.21           | 11               |              | 8.63           | 0.81             | 11               |
|              | 803.03         | 755.73           | 5                |              | 8.13           | 0.55             | 5                |
|              | 1193.96        | 1020.58          | 5                |              | 7.62           | 0.40             | 5                |
|              | 533.20         | 800.76           | 7                |              | 8.44           | 0.74             | 7                |
|              | 1065.66        | 1146.64          | 9                |              | 8.50           | 1.00             | 9                |
|              | 12.50          | 21.53            | 4                |              | 9.50           | 0.35             | 4                |
|              | 809.48         | 1118.84          | 4                |              | 8.40           | 1.06             | 4                |
|              | 73.82          | 289.37           | 7                |              | 8.06           | 1.02             | 7                |
|              | 243.75         | 422.97           | 11               |              | 8.08           | 0.32             | 11               |
|              | 591.31         | 906.16           | 14               |              | 8.80           | 0.93             | 14               |
|              | 1428.50        | 1117.31          | 4                |              | 7.98           | 1.25             | 4                |
|              | 244.79         | 552.35           | 20               |              | 7.94           | 1.02             | 20               |
|              | 134.18         | 511.41           | 5                |              | 8.59           | 0.76             | 5                |
|              | 211.87         | 503.34           | 9                |              | 8.12           | 1.12             | 9                |
|              | 840.19         | 1005.36          | 25               |              | 8.27           | 0.70             | 25               |
|              | 388.21         | 304.07           | 7                |              | 8.89           | 0.51             | 7                |
|              | 570.76         | 548.83           | 5                |              | 8.26           | 0.16             | 5                |
|              | 231.90         | 395.92           | 7                |              | 8.83           | 0.61             | 7                |
|              | 871.76         | 823.57           | 19               |              | 8.05           | 0.51             | 19               |
|              | 1445.32        | 1030.71          | 18               |              | 7.73           | 0.58             | 18               |
|              | 434.01         | 895.48           | 5                |              | 8.33           | 0.69             | 5                |
|              | 927.70         | 514.60           | 6                |              | 8.35           | 0.27             | 6                |
|              | 1300.92        | 1111.42          | 17               |              | 7.97           | 0.74             | 17               |
|              | 341.29         | 691.18           | 7                |              | 8.42           | 0.30             | 7                |
|              | 185.37         | 311.36           | 4                |              | 8.80           | 0.39             | 4                |
|              | 474.54         | 610.27           | 13               |              | 8.24           | 0.39             | 13               |
|              | 1419.81        | 1033.84          | 12               |              | 7.71           | 0.56             | 12               |
|              | 464.34         | 570.43           | 16               |              | 8.34           | 0.84             | 16               |
|              | 573.43         | 428.60           | 8                |              | 8.84           | 0.66             | 8                |
|              | 296.95         | 389.41           | 12               |              | 7.81           | 0.82             | 12               |
|              | 292.24         | 448.64           | 20               |              | 9.25           | 0.84             | 20               |
|              | 1428.95        | 617.70           | 6                |              | 7.80           | 0.79             | 6                |
|              | 1917.29        | 1060.52          | 11               |              | 7.75           | 1.00             | 11               |
|              | 147.19         | 147.26           | 7                |              | 8.93           | 0.41             | 7                |
|              | 233.75         | 375.63           | 6                |              | 8.33           | 0.58             | 6                |
|              | 238.36         | 590.28           | 5                |              | 8.89           | 1.08             | 5                |
|              | 788.48         | 737.93           | 14               |              | 7.96           | 0.53             | 14               |
|              | 648.31         | 518.15           | 13               |              | 8.32           | 0.41             | 13               |
|              | 858.91         | 897.79           | 13               |              | 8.20           | 0.63             | 13               |
|              | 329.35         | 257.23           | 7                |              | 8.79           | 0.35             | 7                |
|              | 8.93           | 41.58            | 4                |              | 10.32          | 0.34             | 4                |
|              | 181.14         | 400.04           | 13               |              | 9.44           | 1.01             | 13               |
|              | 603.60         | 1036.06          | 4                |              | 8.24           | 0.55             | 4                |
|              | 459.95         | 507.47           | 19               |              | 8.31           | 0.39             | 19               |
|              | 235.36         | 266.56           | 6                |              | 8.26           | 0.29             | 6                |
|              | 523.62         | 367.16           | 21               |              | 8.61           | 0.60             | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 1200.000                                                         | 809.649                 | 390.351                     | 8.180                                                            | 8.358                   | -0.178                      |
| 1370.000                                                         | 870.791                 | 499.209                     | 8.150                                                            | 8.352                   | -0.202                      |
| 218.000                                                          | 903.878                 | -685.878                    | 8.720                                                            | 8.359                   | 0.361                       |
| 521.000                                                          | 591.004                 | -70.004                     | 8.500                                                            | 8.563                   | -0.063                      |
| 400.000                                                          | 655.317                 | -255.317                    | 8.850                                                            | 8.416                   | 0.434                       |
| 465.000                                                          | 636.018                 | -171.018                    | 8.520                                                            | 8.450                   | 0.070                       |
| 200.000                                                          | 609.795                 | -409.795                    | 9.050                                                            | 8.548                   | 0.502                       |
| 1340.000                                                         | 639.713                 | 700.287                     | 8.280                                                            | 8.536                   | -0.256                      |
| 65.000                                                           | 430.164                 | -365.164                    | 9.180                                                            | 8.889                   | 0.291                       |
| 730.000                                                          | 433.077                 | 296.923                     | 8.800                                                            | 8.755                   | 0.045                       |
| 200.000                                                          | 440.114                 | -240.114                    | 10.200                                                           | 8.663                   | 1.537                       |
| 2.490                                                            | 216.707                 | -214.217                    | 10.380                                                           | 9.532                   | 0.848                       |
| 103.000                                                          | 447.579                 | -344.579                    | 8.520                                                            | 8.380                   | 0.140                       |
| 260.000                                                          | 684.664                 | -424.664                    | 8.400                                                            | 8.632                   | -0.232                      |
| 200.000                                                          | 569.280                 | -369.280                    | 8.420                                                            | 8.452                   | -0.032                      |
| 24.500                                                           | 479.207                 | -454.707                    | 9.350                                                            | 8.683                   | 0.667                       |
| 360.000                                                          | 971.286                 | -611.286                    | 8.520                                                            | 8.138                   | 0.382                       |
| 200.000                                                          | 1084.233                | -884.233                    | 8.050                                                            | 7.988                   | 0.062                       |
| 1100.000                                                         | 1053.445                | 46.555                      | 7.400                                                            | 7.983                   | -0.583                      |
| 3100.000                                                         | 1202.642                | 1897.358                    | 7.200                                                            | 7.991                   | -0.791                      |
| 50.900                                                           | 247.577                 | -196.677                    | 6.950                                                            | 7.984                   | -1.034                      |
| 190.000                                                          | 411.541                 | -221.541                    | 8.150                                                            | 8.374                   | -0.224                      |
| 200.000                                                          | 610.692                 | -410.692                    | 8.350                                                            | 8.269                   | 0.081                       |
| 32.700                                                           | 383.106                 | -350.406                    | 7.850                                                            | 8.273                   | -0.423                      |
| 1500.000                                                         | 944.818                 | 555.182                     | 7.910                                                            | 8.078                   | -0.168                      |
| 6.100                                                            | 451.328                 | -445.228                    | 9.620                                                            | 8.939                   | 0.681                       |
| 1650.000                                                         | 1237.152                | 412.848                     | 7.460                                                            | 7.972                   | -0.512                      |
| 12.500                                                           | 489.792                 | -477.292                    | 8.920                                                            | 8.305                   | 0.615                       |
| 2380.000                                                         | 1147.982                | 1232.018                    | 6.950                                                            | 8.025                   | -1.075                      |
| 2500.000                                                         | 1192.603                | 1307.397                    | 7.500                                                            | 8.033                   | -0.533                      |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.7652</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.8598</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.58</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.74</b> |
| <b>Variance de la variable Ca à expliquer</b>                    |                         | <b>679352.3</b>             | <b>Variance de la variable pH à expliquer</b>                    |                         | <b>0.6853808</b>            |
| <b>Variance des résidus</b>                                      |                         | <b>395522.8</b>             | <b>Variance des résidus</b>                                      |                         | <b>0.3132309</b>            |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>628.906</b>              | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>0.5596703</b>            |
| <b>WA-PLS : 2 components, SEP = 723</b>                          |                         | <b>R = 0.8873</b>           | <b>WA-PLS : 5 components, SEP = 0.5</b>                          |                         | <b>R = 0.9910</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.78</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.98</b> |
|                                                                  |                         | <b>r = 0.60</b>             |                                                                  |                         | <b>r = 0.71</b>             |



| Water Depth (cm) |                |                  |                  | SO4-- (mg/l) |                |                  |                  |
|------------------|----------------|------------------|------------------|--------------|----------------|------------------|------------------|
| <i>codes</i>     | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|                  | 25.67          | 17.34            | 6                |              | 3076.92        | 1110.96          | 6                |
|                  | 87.37          | 29.17            | 7                |              | 1086.05        | 1485.76          | 7                |
|                  | 26.11          | 7.40             | 6                |              | 3344.37        | 2655.90          | 6                |
|                  | 67.16          | 39.49            | 17               |              | 2597.65        | 2315.38          | 17               |
|                  | 57.59          | 39.93            | 7                |              | 1891.93        | 1392.47          | 7                |
|                  | 27.21          | 21.68            | 5                |              | 5429.08        | 1346.65          | 5                |
|                  | 30.23          | 28.93            | 9                |              | 1630.14        | 1850.29          | 9                |
|                  | 45.72          | 37.44            | 21               |              | 6809.94        | 6514.59          | 21               |
|                  | 21.36          | 15.29            | 9                |              | 7057.99        | 8108.55          | 9                |
|                  | 16.13          | 2.09             | 4                |              | 14551.30       | 12160.47         | 4                |
|                  | 40.15          | 34.56            | 8                |              | 305.49         | 687.34           | 8                |
|                  | 64.47          | 39.29            | 7                |              | 3305.58        | 1521.19          | 7                |
|                  | 43.53          | 35.40            | 13               |              | 2286.84        | 2091.15          | 13               |
|                  | 23.03          | 13.65            | 7                |              | 9398.68        | 9766.64          | 7                |
|                  | 26.08          | 16.73            | 5                |              | 4148.31        | 1100.49          | 5                |
|                  | 69.60          | 39.02            | 11               |              | 1008.27        | 2799.18          | 11               |
|                  | 36.56          | 32.41            | 5                |              | 1276.23        | 1276.24          | 5                |
|                  | 92.14          | 23.81            | 5                |              | 1168.87        | 773.41           | 5                |
|                  | 61.50          | 39.97            | 7                |              | 3118.10        | 2558.73          | 7                |
|                  | 53.22          | 39.73            | 9                |              | 1688.03        | 2099.76          | 9                |
|                  | 35.69          | 31.76            | 4                |              | 31.01          | 37.12            | 4                |
|                  | 53.12          | 39.40            | 4                |              | 1100.61        | 1524.19          | 4                |
|                  | 21.08          | 9.86             | 7                |              | 433.10         | 1332.44          | 7                |
|                  | 25.40          | 20.08            | 11               |              | 413.01         | 682.88           | 11               |
|                  | 39.88          | 35.71            | 14               |              | 1972.44        | 2097.02          | 14               |
|                  | 69.70          | 39.02            | 4                |              | 2235.71        | 1622.06          | 4                |
|                  | 24.70          | 20.03            | 20               |              | 2131.15        | 3533.38          | 20               |
|                  | 23.56          | 16.49            | 5                |              | 238.03         | 770.94           | 5                |
|                  | 23.35          | 18.01            | 9                |              | 2616.59        | 7012.43          | 9                |
|                  | 51.25          | 39.16            | 25               |              | 2074.23        | 2163.68          | 25               |
|                  | 16.24          | 2.16             | 7                |              | 13831.40       | 11352.57         | 7                |
|                  | 21.40          | 3.47             | 5                |              | 1473.46        | 1854.03          | 5                |
|                  | 75.99          | 35.93            | 7                |              | 616.91         | 1375.98          | 7                |
|                  | 51.35          | 39.00            | 19               |              | 1853.26        | 1681.74          | 19               |
|                  | 77.21          | 36.07            | 18               |              | 2854.64        | 1770.38          | 18               |
|                  | 81.46          | 33.76            | 5                |              | 425.92         | 687.68           | 5                |
|                  | 53.12          | 33.05            | 6                |              | 3561.97        | 1428.39          | 6                |
|                  | 71.78          | 37.41            | 17               |              | 2617.36        | 1841.58          | 17               |
|                  | 25.12          | 18.42            | 7                |              | 5723.60        | 986.38           | 7                |
|                  | 17.46          | 2.50             | 4                |              | 4223.57        | 2051.06          | 4                |
|                  | 39.06          | 33.72            | 13               |              | 1241.51        | 1528.46          | 13               |
|                  | 85.37          | 31.13            | 12               |              | 2249.66        | 1569.41          | 12               |
|                  | 28.60          | 25.54            | 16               |              | 2425.68        | 5523.68          | 16               |
|                  | 62.55          | 38.67            | 8                |              | 4066.46        | 1230.23          | 8                |
|                  | 36.40          | 31.84            | 12               |              | 2703.45        | 5066.40          | 12               |
|                  | 25.50          | 25.97            | 20               |              | 5042.76        | 6079.36          | 20               |
|                  | 96.22          | 14.93            | 6                |              | 3008.68        | 1053.60          | 6                |
|                  | 85.99          | 30.13            | 11               |              | 3096.90        | 1026.16          | 11               |
|                  | 31.44          | 31.72            | 7                |              | 3878.28        | 2092.21          | 7                |
|                  | 22.34          | 15.71            | 6                |              | 4307.58        | 9477.35          | 6                |
|                  | 23.34          | 19.95            | 5                |              | 1708.62        | 2017.53          | 5                |
|                  | 62.35          | 39.77            | 14               |              | 1219.75        | 1320.91          | 14               |
|                  | 41.56          | 34.99            | 13               |              | 3528.86        | 4783.96          | 13               |
|                  | 45.42          | 37.20            | 13               |              | 1283.33        | 1244.81          | 13               |
|                  | 39.24          | 36.04            | 7                |              | 7900.61        | 6144.05          | 7                |
|                  | 49.76          | 6.80             | 4                |              | 3593.35        | 622.02           | 4                |
|                  | 38.05          | 19.86            | 13               |              | 4569.58        | 2230.61          | 13               |
|                  | 40.39          | 34.87            | 4                |              | 594.93         | 776.31           | 4                |
|                  | 36.60          | 30.16            | 19               |              | 2281.74        | 2523.52          | 19               |
|                  | 24.39          | 17.26            | 6                |              | 417.85         | 605.88           | 6                |
|                  | 27.40          | 27.15            | 21               |              | 13693.55       | 11044.40         | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 30.000                                                           | 48.048                  | -18.048                     | 5700.000                                                         | 3467.345                | 2232.655                    |
| 30.000                                                           | 51.388                  | -21.388                     | 3070.000                                                         | 3516.977                | -446.977                    |
| 100.000                                                          | 53.718                  | 46.282                      | 2300.000                                                         | 3491.296                | -1191.296                   |
| 20.000                                                           | 42.499                  | -22.499                     | 17900.000                                                        | 7575.381                | 10324.619                   |
| 100.000                                                          | 48.317                  | 51.683                      | 4320.000                                                         | 5001.739                | -681.739                    |
| 100.000                                                          | 45.509                  | 54.491                      | 4660.000                                                         | 5550.414                | -890.414                    |
| 20.000                                                           | 43.393                  | -23.393                     | 2600.000                                                         | 5734.399                | -3134.399                   |
| 20.000                                                           | 46.190                  | -26.190                     | 4080.000                                                         | 6263.509                | -2183.509                   |
| 15.000                                                           | 32.839                  | -17.839                     | 5070.000                                                         | 6937.772                | -1867.772                   |
| 15.000                                                           | 23.971                  | -8.971                      | 26600.000                                                        | 11548.886               | 15051.114                   |
| 15.000                                                           | 29.545                  | -14.545                     | 4360.000                                                         | 5405.575                | -1045.575                   |
| 50.000                                                           | 42.387                  | 7.613                       | 3710.000                                                         | 4295.603                | -585.603                    |
| 20.000                                                           | 32.489                  | -12.489                     | 5980.000                                                         | 5253.148                | 726.852                     |
| 20.000                                                           | 50.686                  | -30.686                     | 6440.000                                                         | 3957.202                | 2482.798                    |
| 20.000                                                           | 51.707                  | -31.707                     | 265.000                                                          | 2787.123                | -2522.123                   |
| 100.000                                                          | 63.598                  | 36.402                      | 72.000                                                           | 1061.000                | -989.000                    |
| 20.000                                                           | 58.745                  | -38.745                     | 465.000                                                          | 2484.437                | -2019.437                   |
| 100.000                                                          | 67.860                  | 32.140                      | 250.000                                                          | 2533.728                | -2283.728                   |
| 100.000                                                          | 64.911                  | 35.089                      | 1270.000                                                         | 2736.314                | -1466.314                   |
| 100.000                                                          | 70.009                  | 29.991                      | 2460.000                                                         | 2559.531                | -99.531                     |
| 20.000                                                           | 26.840                  | -6.840                      | 105.000                                                          | 2165.341                | -2060.341                   |
| 20.000                                                           | 33.344                  | -13.344                     | 302.000                                                          | 4186.065                | -3884.065                   |
| 20.000                                                           | 41.007                  | -21.007                     | 305.000                                                          | 2404.631                | -2099.631                   |
| 20.000                                                           | 34.938                  | -14.938                     | 130.000                                                          | 2193.485                | -2063.485                   |
| 20.000                                                           | 55.110                  | -35.110                     | 2920.000                                                         | 2207.240                | 712.760                     |
| 20.000                                                           | 41.971                  | -21.971                     | 14.000                                                           | 1402.441                | -1388.441                   |
| 100.000                                                          | 70.063                  | 29.937                      | 3370.000                                                         | 2777.558                | 592.442                     |
| 20.000                                                           | 36.766                  | -16.766                     | 4.990                                                            | 1957.775                | -1952.785                   |
| 100.000                                                          | 66.741                  | 33.259                      | 3240.000                                                         | 2404.016                | 835.984                     |
| 100.000                                                          | 66.259                  | 33.741                      | 3180.000                                                         | 2383.299                | 796.701                     |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.7413</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.8500</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.55</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.72</b> |
| <b>Variance de la variable Tranche d'eau à expliquer</b>         |                         | <b>1397.806</b>             | <b>Variance de la variable SO4 à expliquer</b>                   |                         | <b>2.94E+07</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>836.4213</b>             | <b>Variance des résidus</b>                                      |                         | <b>1.41E+07</b>             |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>28.92095</b>             | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>3750.238</b>             |
| <b>WA-PLS : 2 components, SEP = 41</b>                           |                         | <b>R = 0.8648</b>           | <b>WA-PLS : 5 components, SEP = 3537</b>                         |                         | <b>R = 0.9917</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.74</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.98</b> |
|                                                                  |                         | <b>r = 0.41</b>             |                                                                  |                         | <b>r = 0.76</b>             |

| Cl- (mg/l)   |                |                  |                  | Lithium (mg/l) |                |                  |                  |
|--------------|----------------|------------------|------------------|----------------|----------------|------------------|------------------|
| <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i>   | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|              | 14993.11       | 20451.81         | 6                |                | 58.45          | 111.05           | 6                |
|              | 23639.56       | 33514.01         | 7                |                | 166.63         | 262.07           | 7                |
|              | 15569.22       | 7225.07          | 6                |                | 34.52          | 11.72            | 6                |
|              | 72787.46       | 60379.97         | 17               |                | 490.04         | 456.92           | 17               |
|              | 72700.10       | 65890.75         | 7                |                | 489.38         | 481.26           | 7                |
|              | 37967.34       | 27712.32         | 5                |                | 107.90         | 88.53            | 5                |
|              | 19267.58       | 48614.77         | 9                |                | 147.96         | 406.09           | 9                |
|              | 24130.00       | 20875.09         | 21               |                | 117.22         | 153.79           | 21               |
|              | 19628.20       | 16419.76         | 9                |                | 48.22          | 42.67            | 9                |
|              | 23215.80       | 20889.64         | 4                |                | 15.76          | 12.78            | 4                |
|              | 5807.30        | 16248.26         | 8                |                | 31.95          | 81.62            | 8                |
|              | 10938.92       | 9193.09          | 7                |                | 36.21          | 26.45            | 7                |
|              | 16042.57       | 20076.66         | 13               |                | 77.18          | 144.18           | 13               |
|              | 33282.25       | 23423.09         | 7                |                | 70.51          | 76.11            | 7                |
|              | 10540.70       | 8016.47          | 5                |                | 15.35          | 13.76            | 5                |
|              | 31637.72       | 61943.40         | 11               |                | 231.40         | 479.69           | 11               |
|              | 49128.13       | 53852.89         | 5                |                | 329.55         | 366.88           | 5                |
|              | 69660.26       | 65760.14         | 5                |                | 574.26         | 562.33           | 5                |
|              | 46050.76       | 53391.00         | 7                |                | 238.19         | 328.66           | 7                |
|              | 65349.60       | 72704.67         | 9                |                | 403.86         | 455.04           | 9                |
|              | 286.94         | 864.62           | 4                |                | 1.86           | 5.67             | 4                |
|              | 51973.35       | 72683.44         | 4                |                | 391.45         | 547.51           | 4                |
|              | 3568.51        | 19498.65         | 7                |                | 21.70          | 142.62           | 7                |
|              | 12221.71       | 27972.67         | 11               |                | 78.36          | 169.18           | 11               |
|              | 38783.57       | 62138.53         | 14               |                | 234.57         | 392.79           | 14               |
|              | 94506.10       | 73370.53         | 4                |                | 684.15         | 545.30           | 4                |
|              | 16210.28       | 37029.64         | 20               |                | 87.80          | 254.26           | 20               |
|              | 7456.06        | 32517.56         | 5                |                | 40.63          | 177.12           | 5                |
|              | 11373.54       | 34209.47         | 9                |                | 48.48          | 199.27           | 9                |
|              | 51249.82       | 64592.64         | 25               |                | 354.27         | 488.55           | 25               |
|              | 23962.93       | 19259.33         | 7                |                | 29.68          | 21.89            | 7                |
|              | 22025.46       | 26822.35         | 5                |                | 133.68         | 191.39           | 5                |
|              | 5919.56        | 8371.95          | 7                |                | 27.65          | 36.36            | 7                |
|              | 50956.84       | 52497.13         | 19               |                | 343.67         | 366.05           | 19               |
|              | 98857.86       | 64366.08         | 18               |                | 643.94         | 510.25           | 18               |
|              | 24428.40       | 56771.34         | 5                |                | 197.62         | 482.28           | 5                |
|              | 13756.07       | 6121.92          | 6                |                | 24.21          | 10.55            | 6                |
|              | 86499.48       | 70530.56         | 17               |                | 549.66         | 537.87           | 17               |
|              | 40356.13       | 36909.32         | 7                |                | 170.07         | 337.54           | 7                |
|              | 11904.31       | 12867.56         | 4                |                | 52.48          | 42.71            | 4                |
|              | 24349.91       | 42594.55         | 13               |                | 131.35         | 230.65           | 13               |
|              | 93201.18       | 68176.38         | 12               |                | 613.43         | 500.96           | 12               |
|              | 23300.64       | 38014.12         | 16               |                | 139.97         | 261.14           | 16               |
|              | 13999.22       | 9801.08          | 8                |                | 33.29          | 33.36            | 8                |
|              | 11111.16       | 17226.60         | 12               |                | 50.05          | 105.49           | 12               |
|              | 14437.85       | 30423.25         | 20               |                | 70.78          | 201.00           | 20               |
|              | 112249.90      | 49845.83         | 6                |                | 568.25         | 252.74           | 6                |
|              | 125270.74      | 67082.82         | 11               |                | 860.92         | 551.53           | 11               |
|              | 6736.76        | 7800.39          | 7                |                | 37.07          | 33.10            | 7                |
|              | 13728.14       | 28535.13         | 6                |                | 41.14          | 128.41           | 6                |
|              | 10814.46       | 38052.54         | 5                |                | 56.56          | 207.94           | 5                |
|              | 44325.84       | 49602.85         | 14               |                | 309.45         | 356.24           | 14               |
|              | 25510.28       | 24406.43         | 13               |                | 152.19         | 183.42           | 13               |
|              | 48898.94       | 56756.38         | 13               |                | 362.75         | 457.35           | 13               |
|              | 13299.95       | 9791.01          | 7                |                | 66.50          | 48.26            | 7                |
|              | 4654.01        | 1288.13          | 4                |                | 54.07          | 8.05             | 4                |
|              | 27943.74       | 35632.36         | 13               |                | 122.35         | 156.06           | 13               |
|              | 34312.12       | 66225.71         | 4                |                | 279.98         | 563.92           | 4                |
|              | 13291.57       | 16382.25         | 19               |                | 52.33          | 118.69           | 19               |
|              | 7145.56        | 3654.46          | 6                |                | 43.42          | 24.42            | 6                |
|              | 28007.31       | 24131.16         | 21               |                | 92.79          | 173.32           | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>ESTIMATIONS</i> | <i>and RESIDUS</i>          |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|--------------------|-----------------------------|
| 22000.000                                                        | 16382.306               | 5617.694                    | 25.500                                                           | 49.242             | -23.742                     |
| 13900.000                                                        | 15258.410               | -1358.410                   | 11.800                                                           | 37.755             | -25.955                     |
| 6460.000                                                         | 17306.295               | -10846.295                  | 36.500                                                           | 52.718             | -16.218                     |
| 24600.000                                                        | 24605.609               | -5.609                      | 122.000                                                          | 115.566            | 6.434                       |
| 14500.000                                                        | 29036.055               | -14536.055                  | 37.000                                                           | 158.964            | -121.964                    |
| 15300.000                                                        | 29399.520               | -14099.520                  | 109.000                                                          | 164.771            | -55.771                     |
| 10300.000                                                        | 25460.934               | -15160.934                  | 47.000                                                           | 129.877            | -82.877                     |
| 38700.000                                                        | 26699.959               | 12000.041                   | 176.000                                                          | 137.293            | 38.707                      |
| 2250.000                                                         | 27770.922               | -25520.922                  | 19.500                                                           | 130.516            | -111.016                    |
| 44000.000                                                        | 24015.320               | 19984.680                   | 22.500                                                           | 61.906             | -39.406                     |
| 1970.000                                                         | 25116.932               | -23146.932                  | 2.750                                                            | 130.094            | -127.344                    |
| 4540.000                                                         | 27219.348               | -22679.348                  | 54.100                                                           | 137.076            | -82.976                     |
| 29500.000                                                        | 35892.352               | -6392.352                   | 86.800                                                           | 175.138            | -88.338                     |
| 65000.000                                                        | 51764.414               | 13235.586                   | 196.000                                                          | 301.824            | -105.824                    |
| 7240.000                                                         | 30018.563               | -22778.563                  | 42.500                                                           | 192.471            | -149.971                    |
| 699.000                                                          | 28448.877               | -27749.877                  | 4.800                                                            | 202.218            | -197.418                    |
| 16700.000                                                        | 60321.617               | -43621.617                  | 117.000                                                          | 399.189            | -282.189                    |
| 8060.000                                                         | 67867.867               | -59807.867                  | 52.500                                                           | 453.979            | -401.479                    |
| 61400.000                                                        | 65206.918               | -3806.918                   | 500.000                                                          | 442.065            | 57.935                      |
| 194000.000                                                       | 77789.156               | 116210.844                  | 1640.000                                                         | 522.698            | 1117.302                    |
| 90.200                                                           | 13854.553               | -13764.353                  | 0.507                                                            | 72.611             | -72.104                     |
| 6750.000                                                         | 20275.330               | -13525.330                  | 42.500                                                           | 101.736            | -59.236                     |
| 8310.000                                                         | 34917.531               | -26607.531                  | 57.500                                                           | 221.704            | -164.204                    |
| 600.000                                                          | 19036.701               | -18436.701                  | 3.890                                                            | 111.431            | -107.541                    |
| 85900.000                                                        | 57354.555               | 28545.445                   | 600.000                                                          | 381.853            | 218.147                     |
| 63.200                                                           | 27945.895               | -27882.695                  | 0.347                                                            | 176.855            | -176.508                    |
| 134000.000                                                       | 83734.867               | 50265.133                   | 675.000                                                          | 536.504            | 138.496                     |
| 150.000                                                          | 29453.436               | -29303.436                  | 1.180                                                            | 190.823            | -189.643                    |
| 154000.000                                                       | 75271.078               | 78728.922                   | 1160.000                                                         | 503.956            | 656.044                     |
| 158000.000                                                       | 77381.148               | 80618.852                   | 861.000                                                          | 509.584            | 351.416                     |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.8132</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                    | <b>R = 0.77</b>             |
|                                                                  |                         | <b>R<sup>2</sup> = 0.66</b> |                                                                  |                    | <b>R<sup>2</sup> = 0.59</b> |
| <b>Variance de la variable CI à expliquer</b>                    |                         | <b>2.80E+09</b>             | <b>Variance de la variable Li à expliquer</b>                    |                    | <b>149337.2</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>1.42E+09</b>             | <b>Variance des résidus</b>                                      |                    | <b>79096.27</b>             |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>37698.6</b>              | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                    | <b>281.2406</b>             |
| <b>WA-PLS : 2 components, SEP = 35726</b>                        |                         | <b>R = 0.8823</b>           | <b>WA-PLS : 2 components, SEP = 266</b>                          |                    | <b>R = 0.8739</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.79</b> |                                                                  |                    | <b>R<sup>2</sup> = 0.76</b> |
|                                                                  |                         |                             |                                                                  |                    | <b>r = 0.68</b>             |

| Boron (mg/l) |                |                  |                  | Si (mg/l)    |                |                  |                  |
|--------------|----------------|------------------|------------------|--------------|----------------|------------------|------------------|
| <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> | <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|              | 84.66          | 79.84            | 6                |              | 30.98          | 3.13             | 6                |
|              | 108.74         | 139.96           | 7                |              | 23.06          | 7.45             | 7                |
|              | 96.98          | 59.88            | 6                |              | 34.23          | 13.01            | 6                |
|              | 309.41         | 252.11           | 17               |              | 28.32          | 7.54             | 17               |
|              | 288.37         | 276.56           | 7                |              | 29.37          | 6.22             | 7                |
|              | 374.34         | 237.75           | 5                |              | 34.65          | 11.35            | 5                |
|              | 128.41         | 227.70           | 9                |              | 32.39          | 13.05            | 9                |
|              | 208.90         | 166.22           | 21               |              | 28.86          | 5.78             | 21               |
|              | 265.04         | 285.04           | 9                |              | 27.54          | 7.02             | 9                |
|              | 523.20         | 439.22           | 4                |              | 24.42          | 6.88             | 4                |
|              | 22.06          | 50.54            | 8                |              | 40.50          | 11.41            | 8                |
|              | 141.29         | 62.67            | 7                |              | 29.33          | 6.44             | 7                |
|              | 96.48          | 92.71            | 13               |              | 35.18          | 12.38            | 13               |
|              | 422.29         | 375.90           | 7                |              | 33.12          | 10.08            | 7                |
|              | 122.73         | 35.56            | 5                |              | 27.18          | 8.94             | 5                |
|              | 135.42         | 272.93           | 11               |              | 35.71          | 7.47             | 11               |
|              | 169.76         | 182.32           | 5                |              | 30.16          | 4.95             | 5                |
|              | 330.69         | 324.31           | 5                |              | 23.93          | 8.64             | 5                |
|              | 217.52         | 171.69           | 7                |              | 31.63          | 6.02             | 7                |
|              | 241.04         | 271.12           | 9                |              | 24.72          | 7.73             | 9                |
|              | 1.60           | 3.06             | 4                |              | 20.53          | 8.87             | 4                |
|              | 184.32         | 256.95           | 4                |              | 20.77          | 5.84             | 4                |
|              | 22.74          | 84.07            | 7                |              | 28.97          | 7.48             | 7                |
|              | 45.66          | 97.59            | 11               |              | 39.74          | 13.48            | 11               |
|              | 136.34         | 213.21           | 14               |              | 23.63          | 7.74             | 14               |
|              | 328.98         | 256.78           | 4                |              | 18.42          | 5.28             | 4                |
|              | 107.12         | 171.49           | 20               |              | 33.42          | 9.42             | 20               |
|              | 25.78          | 107.02           | 5                |              | 25.09          | 5.73             | 5                |
|              | 111.57         | 268.04           | 9                |              | 28.51          | 7.73             | 9                |
|              | 231.93         | 275.46           | 25               |              | 26.87          | 7.25             | 25               |
|              | 465.68         | 440.31           | 7                |              | 30.04          | 12.48            | 7                |
|              | 94.53          | 105.20           | 5                |              | 32.15          | 2.98             | 5                |
|              | 30.12          | 53.74            | 7                |              | 31.05          | 9.75             | 7                |
|              | 218.55         | 207.91           | 19               |              | 28.89          | 7.11             | 19               |
|              | 416.32         | 267.21           | 18               |              | 28.74          | 8.61             | 18               |
|              | 112.65         | 277.83           | 5                |              | 27.55          | 8.81             | 5                |
|              | 113.56         | 31.92            | 6                |              | 32.60          | 7.49             | 6                |
|              | 382.55         | 300.96           | 17               |              | 35.51          | 27.28            | 17               |
|              | 321.62         | 183.27           | 7                |              | 33.82          | 4.47             | 7                |
|              | 87.60          | 109.44           | 4                |              | 32.01          | 0.79             | 4                |
|              | 94.87          | 135.43           | 13               |              | 42.62          | 13.73            | 13               |
|              | 363.02         | 282.07           | 12               |              | 26.53          | 7.73             | 12               |
|              | 139.56         | 222.38           | 16               |              | 32.68          | 11.94            | 16               |
|              | 141.03         | 75.15            | 8                |              | 29.13          | 9.85             | 8                |
|              | 114.33         | 193.31           | 12               |              | 34.67          | 11.24            | 12               |
|              | 174.68         | 247.15           | 20               |              | 25.35          | 8.96             | 20               |
|              | 347.25         | 140.06           | 6                |              | 38.52          | 24.37            | 6                |
|              | 509.18         | 272.62           | 11               |              | 31.86          | 25.16            | 11               |
|              | 65.00          | 92.58            | 7                |              | 29.33          | 5.77             | 7                |
|              | 169.14         | 343.71           | 6                |              | 33.55          | 14.67            | 6                |
|              | 83.02          | 131.40           | 5                |              | 24.26          | 5.81             | 5                |
|              | 183.99         | 198.35           | 14               |              | 26.58          | 7.08             | 14               |
|              | 144.36         | 111.20           | 13               |              | 32.49          | 10.28            | 13               |
|              | 203.25         | 259.98           | 13               |              | 35.19          | 11.17            | 13               |
|              | 128.32         | 100.06           | 7                |              | 28.40          | 3.60             | 7                |
|              | 139.13         | 21.03            | 4                |              | 157.05         | 21.14            | 4                |
|              | 275.44         | 228.50           | 13               |              | 100.98         | 61.14            | 13               |
|              | 160.96         | 324.66           | 4                |              | 39.52          | 11.43            | 4                |
|              | 90.54          | 104.74           | 19               |              | 31.12          | 5.17             | 19               |
|              | 28.32          | 16.29            | 6                |              | 45.05          | 13.00            | 6                |
|              | 421.25         | 397.04           | 21               |              | 27.18          | 9.22             | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              | <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|------------------------------------------------------------------|-------------------------|-----------------------------|
| 150.000                                                          | 123.807                 | 26.193                      | 25.200                                                           | 32.419                  | -7.219                      |
| 77.000                                                           | 120.656                 | -43.656                     | 41.400                                                           | 32.550                  | 8.850                       |
| 125.000                                                          | 128.298                 | -3.298                      | 28.600                                                           | 32.431                  | -3.831                      |
| 235.000                                                          | 233.375                 | 1.625                       | 27.500                                                           | 28.893                  | -1.393                      |
| 145.000                                                          | 194.662                 | -49.662                     | 26.100                                                           | 30.078                  | -3.978                      |
| 238.000                                                          | 209.196                 | 28.804                      | 20.600                                                           | 28.957                  | -8.357                      |
| 57.000                                                           | 192.644                 | -135.644                    | 31.600                                                           | 29.424                  | 2.176                       |
| 250.000                                                          | 208.042                 | 41.958                      | 34.400                                                           | 29.419                  | 4.981                       |
| 13.000                                                           | 271.104                 | -258.104                    | 31.400                                                           | 37.281                  | -5.881                      |
| 959.000                                                          | 384.899                 | 574.101                     | 21.900                                                           | 29.686                  | -7.786                      |
| 147.000                                                          | 228.941                 | -81.941                     | 18.700                                                           | 29.181                  | -10.481                     |
| 143.000                                                          | 256.833                 | -113.833                    | 161.000                                                          | 108.663                 | 52.337                      |
| 263.000                                                          | 274.761                 | -11.761                     | 32.500                                                           | 35.529                  | -3.029                      |
| 612.000                                                          | 307.855                 | 304.145                     | 45.600                                                           | 58.906                  | -13.306                     |
| 29.900                                                           | 164.081                 | -134.181                    | 36.400                                                           | 32.689                  | 3.711                       |
| 3.490                                                            | 123.997                 | -120.507                    | 38.400                                                           | 34.046                  | 4.354                       |
| 60.000                                                           | 265.911                 | -205.911                    | 31.600                                                           | 31.744                  | -0.144                      |
| 28.400                                                           | 298.557                 | -270.157                    | 17.300                                                           | 28.375                  | -11.075                     |
| 290.000                                                          | 297.368                 | -7.368                      | 20.500                                                           | 28.086                  | -7.586                      |
| 944.000                                                          | 336.567                 | 607.433                     | 31.400                                                           | 30.057                  | 1.343                       |
| 0.995                                                            | 103.283                 | -102.288                    | 37.200                                                           | 32.256                  | 4.944                       |
| 25.500                                                           | 175.538                 | -150.038                    | 58.800                                                           | 34.981                  | 23.819                      |
| 32.000                                                           | 179.071                 | -147.071                    | 32.200                                                           | 35.390                  | -3.190                      |
| 2.920                                                            | 114.049                 | -111.129                    | 30.200                                                           | 33.632                  | -3.432                      |
| 320.000                                                          | 248.693                 | 71.307                      | 34.200                                                           | 29.630                  | 4.570                       |
| 0.703                                                            | 115.891                 | -115.188                    | 15.900                                                           | 23.444                  | -7.544                      |
| 404.000                                                          | 349.545                 | 54.455                      | 33.000                                                           | 32.587                  | 0.413                       |
| 1.080                                                            | 149.260                 | -148.180                    | 22.400                                                           | 28.209                  | -5.809                      |
| 545.000                                                          | 314.913                 | 230.087                     | 16.800                                                           | 29.672                  | -12.872                     |
| 520.000                                                          | 324.056                 | 195.944                     | 31.400                                                           | 30.689                  | 0.711                       |
| <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.7577</b>           | <b>WA: Coefficient de corrélation multiple</b>                   |                         | <b>R = 0.9411</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.57</b> |                                                                  |                         | <b>R<sup>2</sup> = 0.88</b> |
| <b>Variance de la variable B à expliquer</b>                     |                         | <b>66730.07</b>             | <b>Variance de la variable Si à expliquer</b>                    |                         | <b>633.5131</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>41769.64</b>             | <b>Variance des résidus</b>                                      |                         | <b>149.972</b>              |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>204.3762</b>             | <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>12.24631</b>             |
| <b>WA-PLS : 1 component</b>                                      |                         |                             | <b>WA-PLS : 3 components, SEP = 16.95</b>                        |                         | <b>R = 0.9812</b>           |
|                                                                  |                         |                             |                                                                  |                         | <b>R<sup>2</sup> = 0.96</b> |
|                                                                  |                         |                             |                                                                  |                         | <b>r = 0.75</b>             |

## Density

| <i>codes</i> | <i>OPTIMUM</i> | <i>TOLERANCE</i> | <i>FREQUENCE</i> |
|--------------|----------------|------------------|------------------|
|              | 1.02           | 0.02             | 6                |
|              | 1.03           | 0.04             | 7                |
|              | 1.02           | 0.01             | 6                |
|              | 1.08           | 0.06             | 17               |
|              | 1.08           | 0.07             | 7                |
|              | 1.05           | 0.03             | 5                |
|              | 1.02           | 0.05             | 9                |
|              | 1.04           | 0.03             | 21               |
|              | 1.03           | 0.03             | 9                |
|              | 1.05           | 0.04             | 4                |
|              | 1.01           | 0.02             | 8                |
|              | 1.02           | 0.01             | 7                |
|              | 1.02           | 0.02             | 13               |
|              | 1.05           | 0.03             | 7                |
|              | 1.02           | 0.01             | 5                |
|              | 1.04           | 0.07             | 11               |
|              | 1.06           | 0.06             | 5                |
|              | 1.08           | 0.07             | 5                |
|              | 1.05           | 0.06             | 7                |
|              | 1.07           | 0.08             | 9                |
|              | 1.00           | 0.00             | 4                |
|              | 1.06           | 0.08             | 4                |
|              | 1.00           | 0.02             | 7                |
|              | 1.01           | 0.03             | 11               |
|              | 1.04           | 0.07             | 14               |
|              | 1.10           | 0.08             | 4                |
|              | 1.02           | 0.04             | 20               |
|              | 1.01           | 0.04             | 5                |
|              | 1.02           | 0.04             | 9                |
|              | 1.06           | 0.07             | 25               |
|              | 1.05           | 0.04             | 7                |
|              | 1.03           | 0.03             | 5                |
|              | 1.01           | 0.01             | 7                |
|              | 1.06           | 0.06             | 19               |
|              | 1.11           | 0.07             | 18               |
|              | 1.03           | 0.06             | 5                |
|              | 1.02           | 0.01             | 6                |
|              | 1.10           | 0.07             | 17               |
|              | 1.05           | 0.04             | 7                |
|              | 1.02           | 0.02             | 4                |
|              | 1.03           | 0.05             | 13               |
|              | 1.10           | 0.07             | 12               |
|              | 1.03           | 0.04             | 16               |
|              | 1.02           | 0.01             | 8                |
|              | 1.02           | 0.02             | 12               |
|              | 1.02           | 0.04             | 20               |
|              | 1.12           | 0.05             | 6                |
|              | 1.14           | 0.07             | 11               |
|              | 1.01           | 0.01             | 7                |
|              | 1.02           | 0.04             | 6                |
|              | 1.01           | 0.04             | 5                |
|              | 1.05           | 0.05             | 14               |
|              | 1.03           | 0.03             | 13               |
|              | 1.06           | 0.06             | 13               |
|              | 1.03           | 0.02             | 7                |
|              | 1.03           | 0.00             | 4                |
|              | 1.05           | 0.03             | 13               |
|              | 1.04           | 0.07             | 4                |
|              | 1.02           | 0.02             | 19               |
|              | 1.01           | 0.00             | 6                |
|              | 1.05           | 0.04             | 21               |

| <i>Observed values</i>                                           | <i>Estimated values</i> | <i>RESIDUS</i>              |
|------------------------------------------------------------------|-------------------------|-----------------------------|
| 1.032                                                            | 1.023                   | 0.009                       |
| 1.020                                                            | 1.022                   | -0.002                      |
| 1.010                                                            | 1.024                   | -0.014                      |
| 1.050                                                            | 1.038                   | 0.012                       |
| 1.022                                                            | 1.039                   | -0.017                      |
| 1.024                                                            | 1.040                   | -0.016                      |
| 1.015                                                            | 1.036                   | -0.021                      |
| 1.051                                                            | 1.038                   | 0.013                       |
| 1.009                                                            | 1.041                   | -0.032                      |
| 1.087                                                            | 1.043                   | 0.044                       |
| 1.008                                                            | 1.035                   | -0.027                      |
| 1.029                                                            | 1.046                   | -0.017                      |
| 1.040                                                            | 1.047                   | -0.007                      |
| 1.081                                                            | 1.065                   | 0.016                       |
| 1.009                                                            | 1.037                   | -0.028                      |
| 1.001                                                            | 1.032                   | -0.031                      |
| 1.020                                                            | 1.069                   | -0.049                      |
| 1.010                                                            | 1.077                   | -0.067                      |
| 1.073                                                            | 1.075                   | -0.002                      |
| 1.211                                                            | 1.087                   | 0.124                       |
| 1.000                                                            | 1.018                   | -0.018                      |
| 1.009                                                            | 1.028                   | -0.019                      |
| 1.010                                                            | 1.042                   | -0.032                      |
| 1.001                                                            | 1.024                   | -0.023                      |
| 1.098                                                            | 1.065                   | 0.033                       |
| 1.000                                                            | 1.032                   | -0.032                      |
| 1.147                                                            | 1.094                   | 0.053                       |
| 1.000                                                            | 1.035                   | -0.035                      |
| 1.167                                                            | 1.084                   | 0.083                       |
| 1.171                                                            | 1.087                   | 0.084                       |
| <b>WA: Coefficient de correlation multiple</b>                   |                         | <b>R = 0.8003</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.64</b> |
| <b>Variance de la variable Densité à expliquer</b>               |                         | <b>3.25E+00</b>             |
| <b>Variance des résidus</b>                                      |                         | <b>1.7</b>                  |
| <b>Ecart-type des résidus = SEP Standard error of prediction</b> |                         | <b>4.1</b>                  |
| <b>WA-PLS : 2 components, SEP = 0.04</b>                         |                         | <b>R = 0.8827</b>           |
|                                                                  |                         | <b>R<sup>2</sup> = 0.78</b> |
|                                                                  |                         | <b>r = 0.70</b>             |