WQEP - A COMPUTER SPREADSHEET PROGRAM TO EVALUATE WATER QUALITY DATA[1]

by

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A flexible spreadsheet Water Quality Evaluation Program (WQEP) has been developed for mining companies, consultants, and regulators to interpret the results of water quality sampling. In order properly to evaluate hydrologic data, unit conversions and chemical calculations are done, quality control checks are needed, and a complete and up-to-date listing of water quality standards is necessary. This process is time consuming and tends not to be done for every sample. This program speeds the process by allowing the input of up to 115 chemical parameters from one sample. WQEP compares concentrations with EPA primary and secondary drinking water MCLs or MCLG, EPA warmwater and coldwater acute and chronic aquatic life criteria, irrigation criteria, livestock criteria, EPA human health criteria, and several other categories of criteria. The spreadsheet allows the input of State or local water standards of interest. Water quality checks include: anion/cations, TDS_m/TDS_c (where m=measured and c=calculated), EC_m/EC_c, EC_m/ion sums, TDS_c/EC ratio, TDS_m/EC, EC vs. alkalinity, two hardness values, and EC vs. Σ cations. WQEP computes the dissolved transport index of 23 parameters, computes ratios of 26 species for trend analysis, calculates non-carbonate alkalinity to adjust the bicarbonate concentration, and calculates 35 interpretive formulas (pE, SAR, S.I., unionized ammonia, ionized sulfide HS-, pK_x values, etc.). Fingerprinting is conducted by automatic generation of stiff diagrams and ion histograms. Mass loading calculations, mass balance calculations, conversions of concentrations, ionic strength, and the activity coefficient and chemical activity of 33 parameters is calculated. This program allows a speedy and thorough evaluation of water quality data from metal mines, coal mining, and natural surface water systems and has been tested against hand calculations.

Key Words: Water Quality, Computer Programs, Chemistry, Coal mining, Mining

Introdnction

The evaluation of water quality data can be just as tedious and time consuming as collecting the data itself. Poor interpretation of data may lead to erroneous decision making. The science of hydrologic data interpretation is a complex and ever changing. New techniques are constantly being developed to evaluate the data.

Some evaluation methods work better for certain types of water characteristics, but not all (See Hem, 1992, and Hounslow, 1995). Other methods may work well but either do not catch on or fall out of favor. Often, the methods of interpretation exist but we do not have the time to apply them to all our analyses. The hydrologist must also possess a diversity of skills to be a good evaluator of data. The task requires one to be an organic chemist, an inorganic chemist, a mathematician, a computer specialist, a statistician, knowledgeable in regulatory standards, experienced with data interpretation and methodology, and possessing good intuition. Unfortunately few of us are this diverse.

A computer program was developed to aid in water data interpretation of single samples. The program is geared toward inorganic constituents with

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some water quantity calculations included. The program is designed to be flexible, easily expanded, and receptive to modification. It does not handle large sets of data; rather, it is designed to look at one or two samples at a time and provide a thorough interpretation. A full suite of chemical analyses is necessary to optimize the program's capability.

Methods

A **W**ater **Q**uality **E**valuation **P**rogram called WQEP has been developed. The program is based on a water quality evaluation program developed in OSM's Kansas City Field Office in 1989 (Liddle, 1989). The program has been continually modified and debugged and has been used in-house on hundreds of sites. The program results were frequently compared with those obtained by hand calculation or other software programs such as Wateq4F (Ball, 1991) and HC-GRAM (McIntosh, 1986). The program was developed for Lotus 1,2,3 spreadsheets and can be converted to other spreadsheet platforms such as Excel.

Lotus was chosen because the program could be easily changed by inexperienced programmers to tailor the model to different regions and ever changing water quality criteria. Lotus can handle small databases depending on the computer's memory and has data transfer capabilities with many other databases such as dBase, FoxPro, Oracle, ParLens, and SQL Server (Bradley, 1994, p. 1028). From a practical standpoint, since the program is designed to analyze full suite water chemistry, the cost of data collection usually limits the number of samples to be analyzed. This makes most databases of full suite water chemistry manageable.

Tedious hydro-chemical calculations were programmed to allow the user to concentrate on the results not the calculations. Data interpretation methods were obtained from numerous publications. Greenberg (1992), Hem (1985), and Minear (1982) provides good discussions about the interpretation techniques. General water quality references showing examples include Benefield (1982), Stumm (1996), Novotny (1994), Manahan (1991), and Bodek (1988). General chemistry calculations can be found in Sawyer (1967). Statistical methods for water resources can be found in Helsel (1992), Koch (1970), Barnes (1994), and Haan (1977). Soil, rock, and water chemistry interrelations are discussed in Loeppert (1995), Stumm (1995), Bohn (1985), and Garrels (1965). The pH concept is explained by Westcott (1978). Case studies, water quality summaries, and hydrologic investigation reports were used to find additional ideas. Examples include Likens (1995) and USGS (1993). Being an avid reader of USGS Water Resources Investigations and Open-File Reports is beneficial in seeing a variety of interpretation techniques and illustrations from many hydrologists.

Model Components

The program conducts several types of quality assurance checks, comparisons with water quality standards, data manipulations, calculation of other parameters, and graphical presentations. WQEP allows the importation of 115 chemical parameters including dissolved and total species; metals and trace elements; conventional pollutants; and physical parameters. They include the following:

acidity	carbonate	lead	phosphate	sulfate
alkalinity	cesium	lithium	potassium	sulfide
aluminum	chloride	magnesium	radium	TDS
ammonia	chromium	manganese	radon	Temp.
antimony	cobalt	mercury	scandium	thallium
arsenic	conduct.	molybdenum	selenium	titanium
barium	copper	nickel	SS	TSS
beryllium	cyanide	nitrate	silica	uranium
bicarb.	fluoride	nitrite	silver	vanadium
boron	gallium	ORP	sodium	yttrium
cadmium	hardness	DO	strontium	zinc
calcium	iron	pH	sulfate	zirconium

The model immediately conducts calculations to predict the value of other species such as un-ionized ammonia, ionized sulfide HS, sulfide (S2-), bicarbonate, hardness, etc.

WQEP runs more than 10 different quality assurance checks to evaluate the quality of the data. Water quality checks include: anion/cations, TDS_m/TDS_c, EC_m/EC_c, EC_m/ion sums, TDS_c/EC ratio, TDS_m/EC, EC vs. alkalinity, two hardness values, EC vs. Σ cations, and ionic strength comparisons.

The program contains the latest water quality criteria, standards, and threshold values cited in the

literature. Federal Register notices were compiled on each parameter to understand the latest regulatory requirements rather than rely on outdated water quality tables.

The program automatically compares each of the 115 chemical parameters to up to 16 categories of criteria and standards. These include:

EPA Drinking Water MCL
EPA Drinking Water MCLG
EPA Secondary Drinking Water MCL
EPA Warmwater Aquatic Criteria
    Chronic
    Acute
EPA Coldwater Aquatic Criteria
    Chronic
    Acute
Irrigation Criteria (various sources)
Livestock Criteria (various sources)
EPA Human Health Criteria
    Water and Organisms
    Organisms Only
National Ambient Levels (Bodek)
State Sediment Criteria
Other State Criteria
Optional Criteria

The program displays a "WARNING!" note beside each parameter that exceeds some water quality criteria and shows which column the parameter exceeded.

Several aquatic life criteria for metals vary depending on the hardness or alkalinity of the receiving stream. The values are derived from regression equations relating the two parameters. The program allows the user to enter a hardness value and the criteria are automatically calculated. The parameters calculated are as follows:

CHRONIC CONCENTRATIONS SHOULD NOT EXCEED:

$$\mu g/l\ Cd = e^{(0.7852\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -3.490}$$

$$\mu g/l\ Cr(III) = e^{(0.8190\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +1.561}$$

$$\mu g/l\ Cu = e^{(0.8545\ [\ 1\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -1.465}$$

$$\mu g/l\ Pb = e^{(1.266\ [\ 1\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -4.661}$$

$$\mu g/l\ Ni = e^{(0.8460\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +1.1645}$$

$$\mu g/l\ Ag = e^{(1.72\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -6.52}$$

$$\mu g/l\ Zn = e^{(0.8473\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +\ 0.7614}$$

more than once every three years on average.

ACUTE CONCENTRATIONS SHOULD NOT EXCEED:

$$\mu g/l\ Cd = e^{(1.128\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -3.828}$$

$$\mu g/l\ Cr(III) = e^{(0.8190\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +3.688}$$

$$\mu g/l\ Cu = e^{(0.9422\ [\ 1\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -1.464}$$

$$\mu g/l\ Pb = e^{(1.266\ [\ 1\ Ln\ (\ Hardness\ mg/l\ )\ ]\ -1.416)}$$

$$\mu g/l\ Ni = e^{(0.8460\ [\ 1\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +3.3612)}$$

$$\mu g/l\ Zn = e^{(0.8473\ [\ Ln\ (\ Hardness\ mg/l\ )\ ]\ +\ 0.8604)}$$

more than once every three years on average.

The program also calculates bicarbonate alkalinity, carbonate, alkalinity, hydroxide alkalinity, free carbon dioxide, and total carbon dioxide, and noncarbonate alkalinity. The dissolved transport index (DTI) (Horowitz, 1991) is calculated for 23 parameters based on the dissolved and total species present in the water. More than 25 different ionic ratios are calculated such as sulfate/TDS, Cu/Mo, Ca/SO_4, etc. The program allows user defined ratios to be calculated.

Index parameters such as ESP, SAR, Morphoedaphic index (Brocksen, 1992), Langelier saturation index, etc. are also calculated. Conversions into equivalents and moles are conducted. Dissociation constants, dielectric constant, pE from eH, and other tedious calculations are automatically done.

The model provides some rough dual species solubility calculations but is not intended to replace hydro geochemical models such as WATEQ4F (Ball, 1991) or Solmineq.88 (Kharaka, 1988). Chemical activities are calculated using the Debye-Huckel ionic strength method. Ion solubility product constants K_{sp} and activity product constants K_{iap} are printed for 56 species.

One additional feature allows the input of a flow measurement in cfs or gpm. This value is used for the mass balance mixing model calculations. Downstream water chemistry can be predicted based on baseline data and the addition of one or more discharges knowing the flow rates.

Mass loading calculations are also calculated in several ways. The program takes the concentration of the constituent such as iron, adjusts for the flow rate, and calculates loading in pounds per day, pounds per year, tons per day, and tons per year. By entering a sediment density value into the program, the potential sediment accumulation is calculated in cubic feet per month and cubic feet per year. This is beneficial for dam and reservoir siltation estimations.

WQEP automatically produces a histogram of major ions and a STIFF diagram for water quality fingerprinting. These graphics along with the normal graphing features of a spreadsheet program allow a quick and effective illustration of data. The nature of a spreadsheet allows additional water evaluation techniques to be added to the program as they are developed with little effort.

Conclusions

A Water Quality Evaluation Program (WQEP) was developed for special use in situations where full suites of major ions, metals, trace elements, and field parameters are collected for individual samples. The program does many water interpretation calculations that are generally too tedious and time consuming to do for every sample. The program enables quality assurance and detailed evaluations to be quickly conducted so that the hydrologist can concentrate on the other aspects of the data.

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