AquaChem
User's Manual

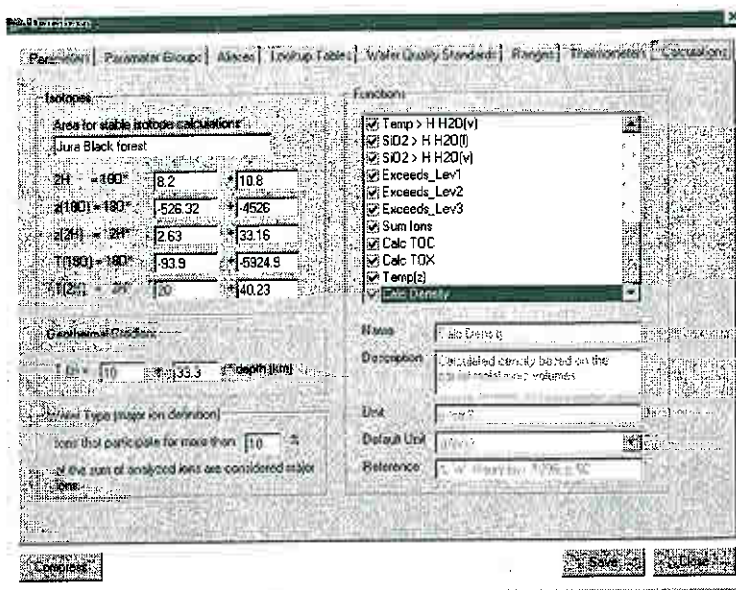## Water Quality Data
Analysis, Plotting, & Modeling

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b in the Database options dialogue is the **Calculations** tab, as shown below:

The **Calculations** tab allows you to set the equation coefficients and parameters that are used in the isotope and geothermometer calculations. It also provides information on the various calculations that are performed by AquaChem.

Isotopes

In the **Isotopes** frame, you may define coefficients for several functions for the isotopic calculations. With the exception of the meteoric water line, all equations have a highly regional character. If you want to make temperature or precipitation estimations, please find the respective coefficients for your study area. There are also parameters for ^{18}O (Oxygen 18) and ^{2}H (deuterium) equations: meteoric waterline, altitude-isotope and altitude-mean annual temperature relations. All of these functions are derived empirically. The coefficients for the isotope-altitude and the isotope-temperature functions are regional and should be used only in the area of calibration. Indicate the area of application of these functions in the field provided.

Geothermal Gradient

The **Geothermal Gradient** is used for a simple subsurface temperature estimation. These options allow you to specify which values are used to calculate the temperature at a given depth. The geothermal gradient is used in the geothermometer plot. It allows

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the user to estimate the subsurface temperature of waters produced by a borehole if the depth of the inflow zone is known. This temperature is then compared to geothermometer temperatures for the respective sample.

The formula for the Geothermal Gradient calculation is as follows:

The subsurface temperature [T (z)] = Average surface temperature + geothermal gradient * depth (km).

The geothermal gradient may vary regionally; it is approximately 33 °C/km in most environments. Any changes made to the Geothermal gradient equation should be registered with AquaChem by pressing the **[Save]** button prior to closing the **Database** options dialogue.

Water Type (major ion definition)

The criterion for determining if an ion is major is normally 10%; however in some places 12.5% is more common. This option allows you to enter a new value for the major ions calculations definition. This will influence the water type calculation which is based on the major ions.

Water type is calculated as follows:

- All concentrations are converted to meq/L.
- Values are then transformed from meq/L to meq%.
- All parameters which are below a certain limit (10% by default) are removed.
- The remaining ions are considered **Major ions**. These ions are ordered according to their percentage. Cations are ordered first, followed by the anions.
- The result is the **WaterType** string (e.g. $Ca-Mg-HCO_3$).

The Water Type is displayed in the **Sample Details** window as a distinct parameter.

NOTE: The Water Type parameter cannot be edited; it is read-only.

Functions

The **Functions** frame lists all of the internal calculations performed by AquaChem, with reference information for each calculation provided in the fields below. All of the active functions (as indicated by a checkmark) will be available as database parameters which can be included in statistical comparisons and for plotting data. In this dialogue, you may select which calculations should appear in the function lists. For example, if you never use the enthalpy calculation, you may deactivate it here. In addition, you may define the default units for some of the functions.

The calculated values are displayed in the **Sample Details** window, under the **Calculated** tab: