

The Geochemist's Workbench

GWB Essentials

The Geochemist's Workbench 15 Essentials edition makes quick work of the tasks most commonly encountered in geochemical modeling. With a few mouse clicks, you can balance reactions, figure equilibrium constants, and produce Eh-pH (Pourbaix) and activity diagrams. The package features a spreadsheet designed to hold and manipulate your geochemical data.

Spreadsheet for Geochemists



Program **GSS** is the Geochemist's spreadsheet, designed to hold and manipulate your chemical analyses. Paste in your data and you can:

- Convert chemical units.
- Compute mineral saturation, gas fugacity.
- Check for charge balance and figure TDS.
- Figure aqueous species distribution, redox state.
- Compare replicates and check standards.
- Produce time series, cross plots, and ternary_plots. Make Piper, Stiff, Durov, ion balance diagrams.



Eh-pH and activity Diagrams

Programs **Act2** and **Tact** produce diagrams showing areas of predominance for aqueous species, and stability ranges of minerals and gases.



Set as axis variables:

- Eh and pH, including Pourbaix diagrams.
- Aqueous species activity.
- Gas fugacity.

You can also make:

- Solubility diagrams.
- Mosaic diagrams.
- Temperature-activity diagrams.

Distribution of Species



SpecE8 Calculates the distribution of mass among aqueous species. Use the program to

- Figure concentrations, activities, activity coefficients.
- Calculate mineral saturation states, gas fugacities.
- Plot Piper, Stiff, Schoeller, ion balance diagrams.
- Apply the "Pitzer equations" for activity coeffiicients.
- Model sorption, ion exchange, surface complexation.

Reaction Balancing



Program **Rxn**

- balances chemical reactions. You can:
- Balance reactions among aqueous species, minerals, and gases.
- Calculate equilibrium constants -- log Ks.
- Figure equilibrium equations.
- Determine equilibrium temperatures.



Is Essentials right for you?

Interested in how geochemical systems evolve? GWB Standard also calculates reaction paths, traces kinetic reactions, and models microbial metabolism and growth. GWB Professional does all this, plus modeling reactive transport in flowing ground and surface water.

GWB Standard

The Geochemist's Workbench 15 Standard edition does everything Essentials can do. Plus it traces irreversible reaction processes in closed and open geochemical systems.



Reaction Paths

Program **React** simulates multi component reaction in closed systems, or those open to mass and heat fluxes. Almost endlessly configurable, you can use **React** to:

- Model water-rock interaction.
- Simulate fluid mixing.
- Polythermal reactions.
- Fixed and sliding activity or fugacity.
- Speciation diagrams.

Kinetic Rate Laws



React can integrate into any reaction model the kinetics of:



- Mineral dissolution and precipitation.
- Complex association and dissociation.
- Sorption and desorption.
- Redox transformations.
- Enzymes and catalysts.
- Gas transfer.

Microbial Reaction and Growth



React is built to model microbial reaction and growth. It can account for:

- Kinetics of microbiallycatalyzed reactions.
- Growth and decay of microbial populations.
- Thermodynamic constraints on reaction.
- Pure cultures and mixed communities.

Is Standard right for you?

Do you need a versatile and powerful toolset for geochemical modeling, but aren't planning on modeling reaction processes or microbial metabolism? You can license GWB

Essentials now and upgrade later for little more than the price differential. Reactive transport modeling in your future? GWB Professional traces one and two dimensional models that simulate how reactions are distributed in flowing ground and surface water.

GWB Professional

The Geochemist's Workbench 15 Professional edition is your choice for reactive transport modeling.

In addition to the capabilities of Essentials and Standard, the Professional edition includes onedimensional and two-dimensional models of reactive and bioreactive transport.

GWB Pro's advanced algorithms and multithreaded design make it ideal for simulating the fate and transport of contaminants in flowing ground and surface water.



Mass and Heat Transport



Programs X1t and X2t model reactive transport in one and two dimensions. The models account for:

- Advection, dispersion, and diffusion.
- Uniform or heterogeneous medium properties.
- Dual porosity (stagnant zone) effects.
- Heat transfer by advection and conduction.

Equilbrium and Kinetic Reactions



X1t and X2t can

incorporate any combination of equilibrium and kinetic reactions:

- Mineral precipitation and dissolution.
- Complexation and dissociation.
- Sorption and desorption.
- Redox transformation.
- Catalysis and enzymes. Bioreactive Transport



Models can account for reactions catalyzed by microbial activity:

- Pure culture and mixed communities.
- Population growth and decay. Thermodynamic effects.



Graphics and Animation



Program Xtplot

renders the results of your modeling.

- Plot any variable against distance or time.
- Color map, color mask, and contour diagrams.
- Animate map view plots.
- Export animations to make video clips

System Requirement

You can install The Geochemist's Workbench[®] 15 <u>Professional, Standard</u>, or <u>Essentials</u> under Windows 10, 8.1, 8, or 7. The vast majority of users should install the 64 bit, rather than the 32 bit version.

You should have a Pentium or later processor, approximately 4 GB of memory, and about 200 MB of available disk space.