

The Geochemist's Workbench

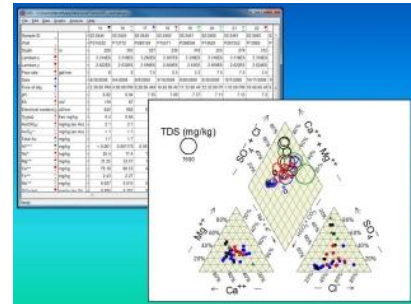
GWB Essentials

The Geochemist's Workbench 9.0 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.



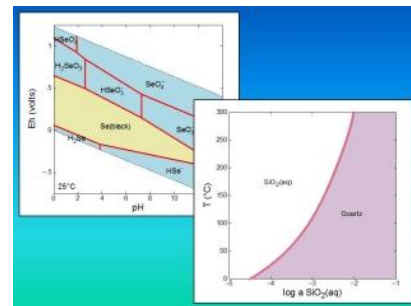
Eh-pH and activity Diagrams

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

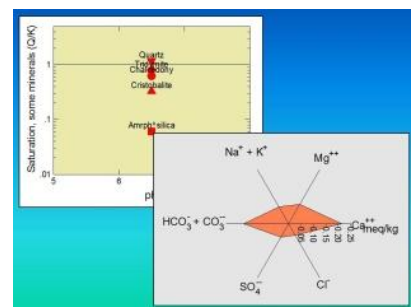
SpecE8 calculates the distribution of mass among aqueous species. Use the program to:

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

Reaction Balancing

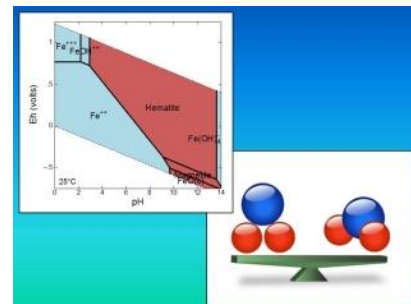
Program **Rxn** balances chemical reactions. You can:

- 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 Version

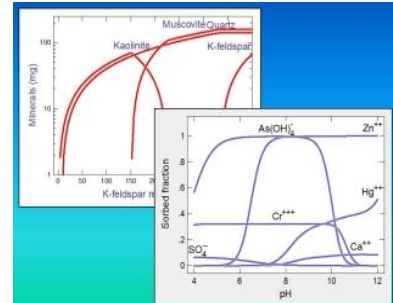
The Geochemist's Workbench 9.0 Standard edition does everything Essentials can do. Plus it traces irreversible reaction processes in closed and open geochemical systems.

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:

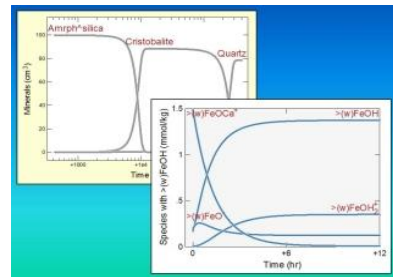
- Model water-rock interaction.
- Simulate fluid mixing.
- Polythermal reactions.
- Fixed and sliding activity or fugacity.
- Speciation diagrams.



Kinetic Rate Laws

React can integrate into any reaction model the kinetics of:

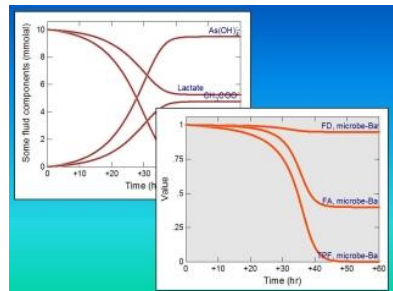
- Mineral dissolution and precipitation.
- Complex association and dissociation.
- Sorption and desorption.
- Redox transformations.
- Enzymes and catalysts.
- Gas transfer.



Microbial Reaction and Growth

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

- Kinetics of microbially catalyzed 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 9.0 Professional edition is your choice for reactive transport modeling.

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

Built for Speed

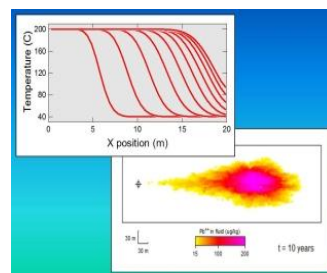


GWB Pro's advanced algorithms and multithreaded design make it ideal for simulating the fate and transport of contaminants in flowing ground and surface water.

Mass and Heat Transport

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

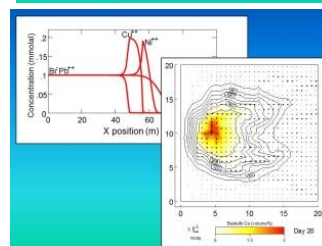
- Advection, dispersion, and diffusion.
- Uniform or heterogeneous medium properties.
- Dual porosity (stagnant zone) effects.
- Heat transfer by advection and conduction.



Equilibrium and Kinetic Reactions

X1t and **X2t** can incorporate any combination of equilibrium and kinetic reactions:

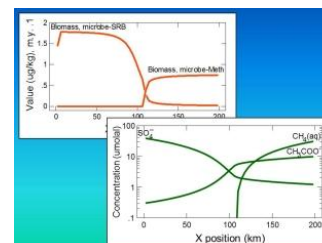
- Mineral precipitation and dissolution.
- Complexation and dissociation.
- Sorption and desorption.
- Redox transformation.
- Catalysis and enzymes.



Bioreactive Transport

Models can account for reactions catalyzed by microbial activity:

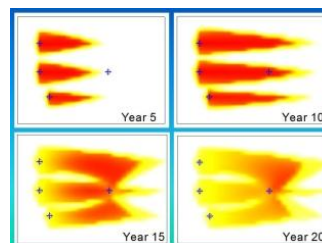
- Pure culture and mixed communities.
- Population growth and decay.
- Thermodynamic effects.



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®** Essentials, Standard, or Professional under Windows 8 or 7 (32 or 64 bit), Windows Vista, or Windows XP. Many of our users run the GWB on a Mac. You should have a Pentium or later processor, approximately 4 GB of memory (2 GB of memory under Windows XP), and about 200 MB of free disk space.

Compare versions

Which version of the GWB is right for you? The chart below shows the programs and features included with each:

Program		Essentials	Standard	Professional
	GSS is a spreadsheet for manipulating and plotting geochemical datasets	✓	✓	✓
	Rxn balances chemical reactions, calculates equilibrium constants, and more	✓	✓	✓
	Act2 generates stability diagrams on activity, Eh, pe, pH, and fugacity axes	✓	✓	✓
	Tact makes temperature-activity and temperature-fugacity diagrams	✓	✓	✓
	SpecE8 figures concentrations of aqueous and sorbed species, saturation, and gas fugacity	✓	✓	✓
	Gtplot displays data from GSS and the results of running SpecE8 and React	✓	✓	✓
	React traces reaction paths involving fluids, minerals, gases, and microbes		✓	✓
	X1t models reactive transport in groundwater flows in one linear or radial coordinate			✓
	X2t simulates reactive transport in two dimensions, including injecting and producing wells			✓
	Xtplot renders and animates the results of X1t and X2t simulations			✓
Feature		Essentials	Standard	Professional
Spreadsheet for geochemical data		✓	✓	✓
Convert chemical units		✓	✓	✓
Time series, cross, and ternary plots		✓	✓	✓
Piper, Stiff, Durov, Schoeller diagrams		✓	✓	✓
Ion balance bar and pie charts		✓	✓	✓
Flag non-compliance		✓	✓	✓
Calculate mineral saturation and gas fugacity		✓	✓	✓
Mix samples		✓	✓	✓
Compare replicates and check standards		✓	✓	✓
Calculate redox state		✓	✓	✓
Check charge balance		✓	✓	✓
Compute TDS		✓	✓	✓
Eh-pH, activity, and fugacity diagrams		✓	✓	✓
Temperature-activity and temperature-fugacity diagrams		✓	✓	✓
Solubility diagrams		✓	✓	✓
Mosaic (ligand speciation) diagrams		✓	✓	✓
Calculate species' concentration and activity coefficients		✓	✓	✓
Redox equilibrium and disequilibrium		✓	✓	✓
Use "Pitzer equations" to compute activity coefficients		✓	✓	✓
Sorption by K_d , Freundlich, and Langmuir models		✓	✓	✓
Ion exchange		✓	✓	✓
Two-layer surface complexation model		✓	✓	✓
Gas and mineral buffering; pH-stat		✓	✓	✓

Balance chemical reactions	✓	✓	✓
Compute equilibrium constants (log K_s) at temperature	✓	✓	✓
Derive equilibrium equations, temperatures	✓	✓	✓
Paste graphs into Word, PowerPoint, Excel, Adobe Illustrator	✓	✓	✓
Save graphics as eps, pdf, ai, emf, svg, and bmp files	✓	✓	✓
Plug-in to other programs	✓	✓	✓
Model water-rock interaction		✓	✓
Simulate fluid mixing		✓	✓
Speciation diagrams vs. pH, etc.		✓	✓
Closed and open chemical systems		✓	✓
Polythermal simulations		✓	✓
Fixed and sliding activity, fugacity		✓	✓
Combine equilibrium and kinetic reactions		✓	✓
Kinetics of mineral precipitation and dissolution		✓	✓
Aqueous complexation and dissociation kinetics		✓	✓
Sorption and desorption kinetics		✓	✓
Kinetics of redox transformation		✓	✓
Enzymes and catalysts		✓	✓
Gas transfer kinetics		✓	✓
Microbial catalysis and growth		✓	✓
Mixed microbial communities		✓	✓
Thermodynamic constraint on microbial metabolism		✓	✓
Specify form of kinetic rate laws		✓	✓
Paste any plot into Excel as numerical data		✓	✓
Reactive and bioreactive transport			✓
Advection, dispersion, and diffusion			✓
Uniform or heterogeneous medium			✓
Dual porosity (stagnant zones)			✓
Advective and conductive heat transfer			✓
Import flow fields			✓
Regular and adaptive grids			✓
Map view, color mask, and contour plots			✓
Animation and output for video			✓