



# Thermodynamic Database Population Software (DBCreate) (20120324, Dr. Martin Saar)

Technology ID

20120324

## Category

Express License

Engineering & Physical

Sciences/Chemicals

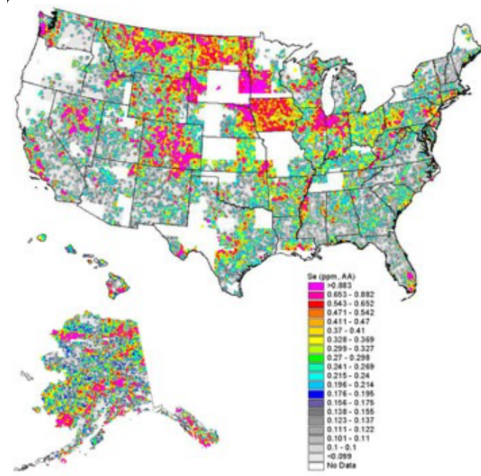
Software & IT/Algorithms

Software & IT/Databases

Software & IT/End User Software

Software & IT/Simulation &

Modeling



## Updates Thermodynamic Databases for Modeling Geochemical Processes

The DBCreate software quickly and accurately updates thermodynamic databases used in geochemical modeling, based on changes in temperatures and pressures. The software facilitates the production of pressure, temperature and problem specific geochemical thermodynamic databases conveniently and quickly while minimizing the possibility of introducing errors caused by manual entry.

## Geochemical Modeling Requires Accurate Thermodynamic Databases

Thermodynamic databases are critical for modeling geochemical processes associated with aqueous species, redox, mineral, and gas solubility reactions. The accuracy of thermodynamic databases directly affects the capability of geochemical models. Therefore, it is essential that the databases are continuously revised and maintained over time as more accurate or revised data becomes available. Geochemical modeling can be found in petroleum engineering, mining, and waste disposal.

The software works with existing thermodynamic database software; specifically Geochemist Work Bench, ToughReact, and EQ3/6. Users enter temperatures and pressures and DBCreate creates the SUPCTR92 formatted reaction (RXN) files and the user-required object database.

## FEATURES AND BENEFITS OF THERMODYNAMIC DATABASE POPULATION SOFTWARE:

- Fast and accurate automated updating of geochemical thermodynamic databases
- Interactive user interface
- Works with Geochemist Work Bench, ToughReact, and EQ3/6 databases
- Applications in petroleum engineering, mining and waste disposal

Learn more



## Negotiable Commercial License for DBCreate

There are variabilities in the commercial license for DBCreate that are best addressed with a conversation. If you are interested in a commercial license please contact the University of Minnesota's [Office for Technology Commercialization](#) with your interests. A Marketing Technology Manager will contact you with further information.

### Researchers

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