SupPHREEQC

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Introduction

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SupPHREEQC is a program written in C++11, which links PHREEQC and SUPCRTBL programs to facilitate geochemical modeling at elevated temperatures and pressures suitable for clastic and carbonate diagenesis, geological carbon storage, and geothermal applications. Users could read the manuscript “SupPHREEQC: A program to generate customized PHREEQC thermodynamic databases from SUPCRTBL and extend calculations to elevated pressures and temperatures” (Zhang et al., in review) for more details. Below, the contents of the software package, compilation, and operation are discussed.

Contents of the Software Package

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Core C++11 source code files:

AqueousModel.h FileInput.h FileOutput.h

Global.h ScreenInput.h ScreenOutput.h

SpeciesMineralGas.h Utility.h

AqueousModel.cpp FileInput.cpp FileOutput.cpp

Global.cpp main.cpp ScreenInput.cpp

ScreenOutput.cpp SpeciesMineralGas.cpp Utility.cpp

C++ library files in folder ‘OtherCppLib’ for 2D scattered data linear interpolation , which are from John Burkardt (<https://people.sc.fsu.edu/~jburkardt/cpp_src/pwl_interp_2d_scattered/pwl_interp_2d_scattered.html>):

pwl\_interp\_2d\_scattered.hpp r8lib.hpp

pwl\_interp\_2d\_scattered.cpp r8lib.cpp

Necessary data files in folder ‘data’:

abnormal gamma.txt

addreplace.txt

addreplace-PHREEQCDAT.txt

bdot vs TP.txt

rxn.dat

SOLUTION\_MASTER\_SPECIES.txt

spronsbl.dat

vmcriticalpoint.txt

kineticsScript.txt

Compiling

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GNU Scientific Library (GSL) is required when compiling. SupPHREEQC has been successfully compiled on Windows 10 and CentOS 7 using GCC.

Running

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cpronsbl.exe and SUPCRTBL.exe are required before running. Their source codes can be downloaded from <https://github.com/HydrogeoIU/SUPCRTBL>.

When running, please place SupPHREEQC.exe, cpronsbl.exe, SUPCRTBL.exe, and folder ‘data’ mentioned above in the same folder. Then run SupPHREEQC.exe and follow the software prompts. The expected PHREEQC thermodynamic databases can be created. For more detailed information, users can read the manuscript Zhang et al. (in review).

Questions Regarding the Software Package

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Questions about the software package could be sent to:

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SupPHREEQC source codes and executable programs can be downloaded from <https://scholarworks.iu.edu/dspace/handle/2022/23355>.