

PACKAGE ID - 000393IBMPC00 PHREEQC

KWIC TITLE - Geochemical Speciation Mass Transfer

AUTHORS - Parkhurst, D.L.
US Geological Survey, Lakewood, CO (United States)

LIMITATION CODE -UNL **AUDIENCE CODE** - UNL

COMPLETION DATE - 01/01/1995 **PUBLICATION DATE** - 01/01/1995

DESCRIPTION - PHREEQC is designed to model geochemical reactions. Based on an ion association aqueous model, PHREEQC can calculate pH, redox potential, and mass transfer as a function of reaction progress. It can be used to describe geochemical processes for both far-field and near-field performance assessment and to evaluate data acquisition needs and test data. It can also calculate the composition of solutions in equilibrium with multiple phases. The data base, including elements, aqueous species, and mineral phases, is independent of the program and is completely user-definable. PHREEQC requires thermodynamic data for each solid, gaseous, or dissolved chemical species being modeled. The two data bases, PREPHR and DEQPAK7, supplied with PHREEQC are for testing purposes only and should not be applied to real problems without first being carefully examined. The conceptual model embodied in PHREEQC is the ion-association model of Pearson and Noronha. In this model a set of mass action equations are established for each ion pair (and controlling solid phases when making mass transfer calculations) along with a set of mass balance equations for each element considered. These sets of equations are coupled using activity coefficient values for each aqueous species and solved using a continued fraction approach for the mass balances combined with a modified Newton-Raphson technique for all other equations. The activity coefficient expressions in PHREEQC include the extended Debye-Huckel, WATEQ Debye-Huckel, and Davies equations from the original United States Geological Survey version of the program. The auxiliary preprocessor program PHTL, which is derived from EQTL, converts EQ3/6 thermodynamic data to PHREEQC format so that the two programs can be compared. PHREEQC can be used to determine solubility limits on the radionuclides present in the waste form. These solubility constraints may be input to the WAPPA leach model.

PACKAGE CONTENTS - Software Abstract; ONWI-435; Media Includes Source, Sample Problems, Documentation, Auxiliary Information, PHREEQC Data Base;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

COMPUTER - IBM PC

OPERATING SYSTEMS - DOS

PACKAGE ID - 000393IBMPC00 PHREEQC

PROGRAMMING LANGUAGES - C

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES -

REFERENCES - David L Parkhurst, User's Guide To PHREEQC, A Computer Program for Speciation, Reaction-path, Advective-transport, and Inverse Geochemical Calculations, 1995.

ABSTRACT STATUS - Abstract first distributed January 1986. CDC CYBER176 version submitted December 1985, distribution limitation removed October 1986. PC version submitted by NEA, tested by NEA. Released Tested 7/26/96.

SUBJECT CLASS CODE - GUPR

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
GEOCHEMISTRY
CHEMICAL REACTIONS
PH VALUE
REDOX POTENTIAL
MASS TRANSFER
PERFORMANCE
WASTE FORMS
RADIOACTIVE WASTE DISPOSAL
THERMODYNAMICS
RADIOISOTOPES
HIGH-LEVEL RADIOACTIVE WASTES
ALPHA-BEARING WASTES
P CODES

EDB SUBJECT CATEGORIES -

990200 052002 400201 580000 540230

SPONSOR - DOE/RW

PACKAGE TYPE - TESTED