

PACKAGE ID - 001146IBMPC00 MINEQL-PC

KWIC TITLE - Chemical Equilibrium Composition of Aqueous
Systems

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

COMPLETION DATE - 01/01/1996 **PUBLICATION DATE** - 11/21/1986

DESCRIPTION - MINEQL is a subroutine package to calculate equilibrium
composition of an aqueous system, accounting for mass transfer.

PACKAGE CONTENTS - Media Directory; Software Abstract; User's Manual;
Information File (2 pages); Installation Instructions (1 page);
Media Includes Source Code, Executable File, Test Case Input and
Output;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - In MINEQL, the Gibbs free energy function is
minimized and mass balance chemical reaction equations are solved
simultaneously.

COMPUTER - IBM PC

OPERATING SYSTEMS - MS DOS 6.0

PROGRAMMING LANGUAGES - FORTRAN-77

SOFTWARE LIMITATIONS - MINEQL does not take into account mass transfer
of water molecules.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - In MINEQL, some treatment of ion exchange is
included.

HARDWARE REQS - The program was tested at NEA-Db on a Dell 466/1 66 MHz
PC/80486

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HARDWARE REQS - (CONT)

TIME REQUIREMENTS - NEA-Db compiled the program and executed the test case included in this package on a DELL 466/1 66 MHz PC/80486. Execution time was 1.2 seconds.

REFERENCES - M. Schweingruber, User's Guide for Extended MINEQL (EIR-Version), Standard Subroutine and Data Library Package, Revision 1, November 21, 1986.

ABSTRACT STATUS - Released tested 2/6/97

SUBJECT CLASS CODE - RU

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
M CODES
AQUEOUS SOLUTIONS
MASS TRANSFER
ENTHALPY
MASS BALANCE
ITERATIVE METHODS
THERMODYNAMIC PROPERTIES
COMPUTER CALCULATIONS
FORTRAN
CHEMICAL EFFLUENTS
GEOCHEMISTRY
GROUND WATER
CHEMICAL REACTIONS
CHEMICAL ANALYSIS
SPECIFIC HEAT
FREE ENTHALPY

EDB SUBJECT CATEGORIES -

990200 540230 400201 661300

SPONSOR - NEA

PACKAGE TYPE - TESTED