

PACKAGE ID - 001220D078000 SOLUPLLOT

KWIC TITLE - Calculate and Plot Complex Potential

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

COMPLETION DATE - 01/03/1986 **PUBLICATION DATE** - 12/01/1978

DESCRIPTION - SOLUPLLOT is a program designed to calculate and plot complex potential, pH diagrams and log oxygen activity, pH diagrams for aqueous chemical systems, considering speciation of ligands, from free energy and thermodynamic activity data. These diagrams, commonly referred to as Eh-pH and ao2-pH diagrams, respectively, define areas of predominance in Eh-pH diagrams or ao2-pH space for chemical species of a chemical system at equilibrium. Over an area of predominance, one predominant species is at greater activity than the other species of the system considered. The diagram axes, pH (a measure of hydrogen ion activity) and either Eh or log ao2 (measures of a tendency toward either oxidation or reduction), are parameters commonly applied in describing the chemistry of aqueous systems.

PACKAGE CONTENTS - Media Directory; Software Abstract; User's Guide; ReadMe Files (4 pages); Media Includes Source Code; Sample Problem Input and Output Data, Graphics Auxiliary Programs;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - SOLUPLLOT calculates a diagram involving the speciation of ligands in three general steps. First the speciation of a pH-dependent ligand system, if specified in the input data, is calculated. Since this system is solely pH-dependent, areas of predominance are defined by constant pH lines which divide the diagram vertically into a number of rectangular subsections. Secondly the program calculates the speciation of an Eh-pH-dependent ligand system, if so specified in the input data. This speciation may be represented by vertical, horizontal, and sloping bounds. The initial diagram is now effectively divided into a number of subdiagrams, each representing the intersection of the area of predominance of one Eh-pH dependent ligand species. Finally the program takes each subdiagram separately and calculates the speciation of the main system. within each subdiagram the program actually calculates two speciations, one among all the species in the main system (the solid-aqueous diagram), and one among only the aqueous species (the aqueous species diagram). The main system within a subdiagram includes main system species, all non speciating ions, and the pH-dependent ligand species and the Eh-pH dependent species that are predominant within that subdiagram.

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METHOD OF SOLUTION - (CONT)

COMPUTER - DEC VAX11/780

OPERATING SYSTEMS - Machine dependent

PROGRAMMING LANGUAGES - FORTRAN-IV

SOFTWARE LIMITATIONS - The limits of this model should be taken into account when attempting more specialised calculations. Specifically, since the program first independently calculates ligand speciation, and then calculates main system speciation within each ligand species area of predominance, no interaction among ligand systems (and non-speciating ions) is considered. Therefore, any attempt to calculate a diagram considering both cations and anions as ligand species or ions will not produce a rigorously correct equilibrium diagram. As an example, a calculation with a main system of copper species and ligand systems of iron species and sulphur species would not produce species forming iron sulfides would not be considered.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Both Eh-pH and aO₂-pH can be calculated.

OTHER PROG/OPER SYS INFO - Most of the program is written in WATFIV and will not run without modification on a standard FORTRAN IV compiler. Extensions of the ANSI standard used in SOLUPLLOT source include in-memory READ and WRITE statements, multiple assignment statements, IF-THEN-DO-ELSE blocks, format free input, multiple statements per card, arithmetic expressions in I/O lists, COMMON block initialization outside of BLOCK DATA subprograms, CHARACTER type statements, character re- placement statements, and relational operators applied to alphanumeric strings. A recent WATFIV manual should be referred to before attempting to translate the program into standard FORTRAN. The graphics portion of the program is written in FORTRAN IV for a G compiler and uses the Graphics Compatibility System (GCS), written at the United States Military Academy, which is generally available at major computer installations. However, any graphic system may be substituted for the GCS since only general functions are utilized (moves, straight line segments, and character output). If the original implementation of GCS is retained, particular attention should be paid to the argument of subroutine USTART. Legal values of this argument depend on the output device to be used and will vary from system to system.

HARDWARE REQS - The program writes to disk, uses a line printer and needs 280K of memory. A Calcomp or Tektronics 4662 plotter are used to create the final output. NEA-DB implemented the program on a VAX-11/780 in 99,840 bytes of main storage for SOLUPLLOT and 73,728 bytes for the auxiliary program. To test the graphics features, a VERSATEC plotter was employed.

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HARDWARE REQS - (CONT)

TIME REQUIREMENTS - Time requirements for job execution at Penn State vary from from under 20 seconds to about 35 seconds depending on the complexity of the chemical system considered. NEA-DB executed the test cases include in the package on VAX-11/780 in 1 minute and 45 seconds of cpu time.

REFERENCES - C.M. Bethke, Program Soluplot, December 1978.

ABSTRACT STATUS - Released tested May 22, 1998.

SUBJECT CLASS CODE - R

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
S CODES
CHEMICAL REACTIONS
PH VALUE
RADIOACTIVE WASTE STORAGE
RADIONUCLIDE MIGRATION

EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/ER

PACKAGE TYPE - TESTED