

**PACKAGE ID** - 000461D0VAX00 SXLSQA

**KWIC TITLE** - For the Interpretation of Solvent Extraction  
Data

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

**COMPLETION DATE** - 01/01/1992   **PUBLICATION DATE** - 01/01/1992

**DESCRIPTION** - SXLSQA models solvent extraction systems involving an acidic and/or a neutral reagent in an organic solvent that can extract from an aqueous solution one or two cations in addition to H plus and one or two anions in addition to OH minus. In modelling data, any number of product species can be assumed to form in either phase. Activity coefficients of species in the aqueous phase can be calculated by the Pitzer treatment and in the organic phase by Hildebrand-Scott treatment.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; Help File for SXLSQA (June 8, 1992); Media Includes Source Code, User's Guide, Linking Instructions, Sample Problem Input and Output;

**SOURCE CODE INCLUDED?** - Yes

**MEDIA QUANTITY** - 1 3.5 Diskette

**METHOD OF SOLUTION** - The observed quantity to be accounted for by the model is calculated for each data point by a short subroutine already provided or, if necessary, one written by the user. This calculation involves the simultaneous solution of N non-linear equations for N specie concentrations using, if necessary, a simplex procedure followed by refinements with a slightly modified core-library subroutine called HYBRD1. The equilibrium constants and other adjustable parameters of the model are then refined by the general least squares subroutine which is a slightly modified version of the program ORGLS. This procedure is repeated for a specified number of refinement cycles or until no significant further improvement in the parameter values is possible.

**COMPUTER** - DEC VAX

**OPERATING SYSTEMS** - VAX

**PROGRAMMING LANGUAGES** - FORTRAN 77

**SOFTWARE LIMITATIONS** - Some FORTRAN compilers do not accept a sufficient number of arguments (as many as 81) for subroutines.

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**SOFTWARE LIMITATIONS - (CONT)**

**SOURCE CODE AVAILABLE (Y/N)** - Y

**UNIQUE FEATURES** - After the user specifies a model and the data, the program determines the size of arrays needed. If necessary, the user can then easily adjust array sizes.

**OTHER PROG/OPER SYS INFO** - The input and output file names are specified by the program. This software is still under development and has not been completely debugged. Users are requested to report any problems they encounter to aid the authors in improving SXLSQA.

**HARDWARE REQS** - The space required by the program depends on the size of the data set and the assumed model. At least 4 Mb of RAM and a math co-processor are recommended.

**TIME REQUIREMENTS** - The running time is similarly dependent on the size of the data set and the number of species assumed in the model. Running times per refinement cycle are typically a few seconds for a model of moderate complexity.

**REFERENCES** - C.F. Baes Jr, Help File For SXLSQA, June 8, 1992\ C.F. Baes Jr, and B.A. Moyer, Solvent Extraction and Ion Exchange, 6, 675-697, 1988; C.F. Baes Jr, W.J. MacDowell, and S.A. Bryan, Solvent Extraction and Ion Exchange, 5, 1-27, 1987; C.F. Baes Jr, B.A. Moyer, G.N. Case, and F.I. Case, Separation Science and Technology, 25, 1675-1688, 1990; W.R. Busing, and H.A. Levy, ORGLS A General FORTRAN Least Squares Program, ORNL-TM-271, 1962; J.H. Hildebrand, and R.L. Scott, The Solubility of Nonelectrolytes, 3rd ed, page 202, 1950; K.S. Pitzer, Activity Coefficients in Electrolyte Solutions Vol 1, 157-208, 1979.

**ABSTRACT STATUS** - Submitted September 1992. Released screened 6/17/96

**SUBJECT CLASS CODE** - U

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
S CODES  
SOLVENT EXTRACTION  
CHEMISTRY  
DATA ANALYSIS  
EQUILIBRIUM  
FORTRAN  
LEAST SQUARE FIT

**EDB SUBJECT CATEGORIES** -

990200 400100

**SPONSOR** - DOE/ER

**PACKAGE TYPE** - SCREENED