

**PACKAGE ID** - 000194MNF00 SOLGASMIXPV

**KWIC TITLE** - Equilibria in Chemical Systems

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

**COMPLETION DATE** - 10/02/1986   **PUBLICATION DATE** - 01/24/1992

**DESCRIPTION** - SOLGASMIX-PV calculates equilibrium relationships in complex chemical systems. Chemical equilibrium calculations involve finding the system composition, within certain constraints, which contains the minimum free energy. The constraints are the preservation of the masses of each element present and either constant pressure or volume. SOLGASMIX-PV can calculate equilibria in systems containing a gaseous phase, condensed phase solutions, and condensed phases of invariant and variable stoichiometry. Either a constant total gas volume or a constant total pressure can be assumed. Unit activities for condensed phases and ideality for solutions are assumed, although nonideal systems can be handled provided activity coefficient relationships are available.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; ORNL/TM-5775;  
Media Includes Source, Sample Problem;

**SOURCE CODE INCLUDED?** - Yes

**MEDIA QUANTITY** - 1 CD Rom

**COMPUTER** - MAINFRAMES

**OPERATING SYSTEMS** - MVS/SP (IBM3084); VMS 4.3 (DEC VAX11)

**PROGRAMMING LANGUAGES** - FORTRAN IV

**SOFTWARE LIMITATIONS** - Maxima of 99 substances, 20 elements and 10 mixtures, where the gas phase is considered a mixture. Each substance is either a gas or a condensed phase species, or a member of a condensed phase mixture.

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

**RELATED SOFTWARE** - SOLGASMIX-PV is based on the earlier SOLGAS and SOLGASMIX codes.

**HARDWARE REQS** - 216 Kbytes of memory are required for execution on an IBM 3084.

**TIME REQUIREMENTS** - Compilation and execution of the sample problem required 2 CPU seconds on an IBM 3084 and 43 CPU seconds on a DEC VAX11/780.

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**TIME REQUIREMENTS - (CONT)**

**REFERENCES** - Theodore M. Besmann, SOLGASMIX-PV, A Computer Program to Calculate Equilibrium Relationships in Complex Chemical Systems, ORNL/TM-5775, April 1977.

**ABSTRACT STATUS** - Abstract first distributed June 1983. IBM360 version submitted May 1979, replaced by IBM3033 version May 1983, replaced October 1988 by revised IBM3033, DEC VAX11 version, sample problem executed by NEADB October 1986 on an IBM3084 and DEC VAX11/780.

**SUBJECT CLASS CODE** - U

**KEYWORDS** -

COMPUTER PROGRAM DOCUMENTATION  
S CODES  
THERMAL EQUILIBRIUM  
CHEMICAL REACTIONS  
STOICHIOMETRY  
GASES

**EDB SUBJECT CATEGORIES** -

990200 400201

**SPONSOR** - DOE/ER

**PACKAGE TYPE** - SCREENED