EQUIL

A PROGRAM FOR COMPUTING CHEMICAL EQUILIBRIA

Reaction Design

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Acknowledgements:

The EQUIL program is a CHEMKIN implementation of the STANJAN program.[1] The original EQUIL program was authored by Andrew E. Lutz, Fran M. Rupley, Robert J. Kee, and W. C. Reynolds.

Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at www.ReactionDesign.com.

EQUIL: A PROGRAM FOR COMPUTING CHEMICAL EQUILIBRIA

ABSTRACT

EQUIL is a program that computes the chemical equilibrium state of an ideal gas or solution mixture. The program provides an interface that accepts input in CHEMKIN format and calls routines in the STANJAN[1] library to find the equilibrium state. STANJAN provides an efficient algorithm for minimizing the free energy of the mixture to find the equilibrium state. EQUIL may run as a stand-alone application, or may be used as a subroutine that can be called from another CHEMKIN application. EQUIL is also designed to handle multiple condensed phases, using SURFACE CHEMKIN to identify non-gas phases.

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1. INTRODUCTION

An established method for evaluating chemical equilibrium is the element-potential method embodied in the Stanford software STANJAN[1] The EQUIL program provides an interface to the STANJAN library of routines, which allows users to specify species and thermodynamic data in CHEMKIN format.

In this version of the equilibrium program, we assume that the gas-phase is a mixture of ideal gases and that condensed phases are ideal solutions. The user selects atomic populations through identity of initial species and their fraction in each phase, as well as the state parameters.

The user may specify the state parameters in a number of different ways, including a) temperature and pressure; b) pressure and entropy; c) enthalpy and pressure; and d) volume and entropy. Species composition can be "frozen" in a given calculation, or the equilibrium composition can be determined. Calculations may be linked through continuations, such that the conditions calculated from a previous equilibrium case can be used as the starting point for a subsequent case with different constraints. In this way, the user can employ EQUIL to analyze stages in a thermodynamic cycle.

For combustion systems, EQUIL can be used to determine adiabatic flame temperatures for constant pressure or constant volume conditions.   To achieve this, one specifies the reactants as the initial species. EQUIL will determine the enthalpy (or energy) of this initial state. Then and equilibrium calculation can be run that includes the combustion products as available species, to which the reactants can be converted. Running a constant pressure and enthalpy (or constant volume and energy) problem using the enthalpy (or energy) of the initial state will thus produce an equilibrium temperature, which is, by definition, the adiabatic flame temperature.

2. THEORY

The basic theory for the element-potential method of determining equilibrium is based on the minimization of Gibbs free energy.   The Gibbs function of a system is:

$$G = \sum_{k=1}^{K} \overline{g}_k N_k \,,$$

(1)

where $\overline{g}_k$ is the partial molal Gibbs function and N_k is the number of moles of each species k in the system. K is the total number of species.

For ideal-gas mixtures or ideal solutions, the partial molal Gibbs functions are given by:

$$\overline{g}_k = g_k(T, P) + RT \ln X_k \,,$$

(2)

where $g_k(T, P)$ is the Gibbs function for the pure species k, evaluated at the system temperature and pressure; R is the universal gas constant; and X_k is the mole fraction of the kth species.

The equilibrium solution at a given temperature and pressure is the distribution of N_k that minimizes the system Gibbs function, G, subject to atomic population constraints (and non-negative N_k). The atomic population constraints are:

$$\sum_{k=1}^{K} n_{jk} N_k = p_j \,, \quad j = 1,...M$$

(3)

where n_{jk} is the number of the jth atoms that appear in the kth molecule, p_j is the total population in moles of the jth atom in the system, and M is the total number of different elements that are present in the system.

Details regarding the relationship between the partial molal Gibbs functions and the elemental potentials for the atoms, as well as the explicit form of the equations solved in the STANJAN library, are described in the STANJAN report.[1]

3.   THE MECHANICS OF USING EQUIL

The CHEMKIN Application User Interface runs the EQUIL program automatically through a mouse-driven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor. The EQUIL program has a modular structure with interfaces to the CHEMKIN Utility package for obtaining kinetic, thermodynamic, and transport parameters. In addition to input directly from the user, EQUIL depends on data obtained from the CHEMKIN Gas-phase and TRANSPORT packages. Therefore, to solve an equilibrium problem the user must first execute the preprocessor programs, "chem" and, optionally, "surf", both of which have access to the thermodynamic database. EQUIL then reads input from the user (described in Chapter 4), solves for equilibrium conditions, and prints the solution. The CHEMKIN Graphical Post-processor can then be launched from the Application User Interface to plot solution data. Figure 1 shows the relationships between these components. For more information about the CHEMKIN Application User Interface or Graphical Post-processor, please see the CHEMKIN Getting Started manual.

The first step is to execute the CHEMKIN Interpreter, "chem". The CHEMKIN Interpreter first reads user-supplied information about the elements and species in a problem. It then extracts further information about the species' thermodynamic properties from a database, (e.g.,"therm.dat"). The user may also optionally input thermodynamic property data directly in the input file to the CHEMKIN Interpreter to override or supplement the database information. The information from the user input and the thermodynamic properties is stored in the CHEMKIN Linking File, "chem.asc"; a file that is later required by the CHEMKIN subroutine library, which will be accessed by the EQUIL program.

If the equilibrium calculation is to consider non gas-phase species, the user must enter this information in a SURFACE CHEMKIN input file and additionally run the SURFACE CHEMKIN Interpreter. The SURFACE CHEMKIN Interpreter will acquire information about "bulk" species. The "bulk" species can be used to describe condensed phases. The Surface Interpreter will also extract further information about the non gas-phase species' thermodynamic properties from the Thermodynamics Database.   Information about the bulk species is stored on the SURFACE CHEMKIN Linking File, "surf.asc", which is then needed by the EQUIL Application. If the EQUIL application does not find a SURFACE CHEMKIN Linking File in the working directory, it will proceed with a gas-phase only equilibrium calculation.

EQUIL makes appropriate calls to the CHEMKIN and the SURFACE CHEMKIN libraries to initialize the species information. The purpose of the initialization is to read the Linking Files and set up the internal working and storage space required by all subroutines in the libraries.

EQUIL reads the input that defines the initial conditions and equilibrium constraints in a Keyword format from the input file (e.g. "equil.inp"). The equilibrium program produces printed output (e.g. "equil.out")

and it saves the solution in a binary Save File, "save.bin". The Save File can be used in post-processing, as described in Chapter 5.
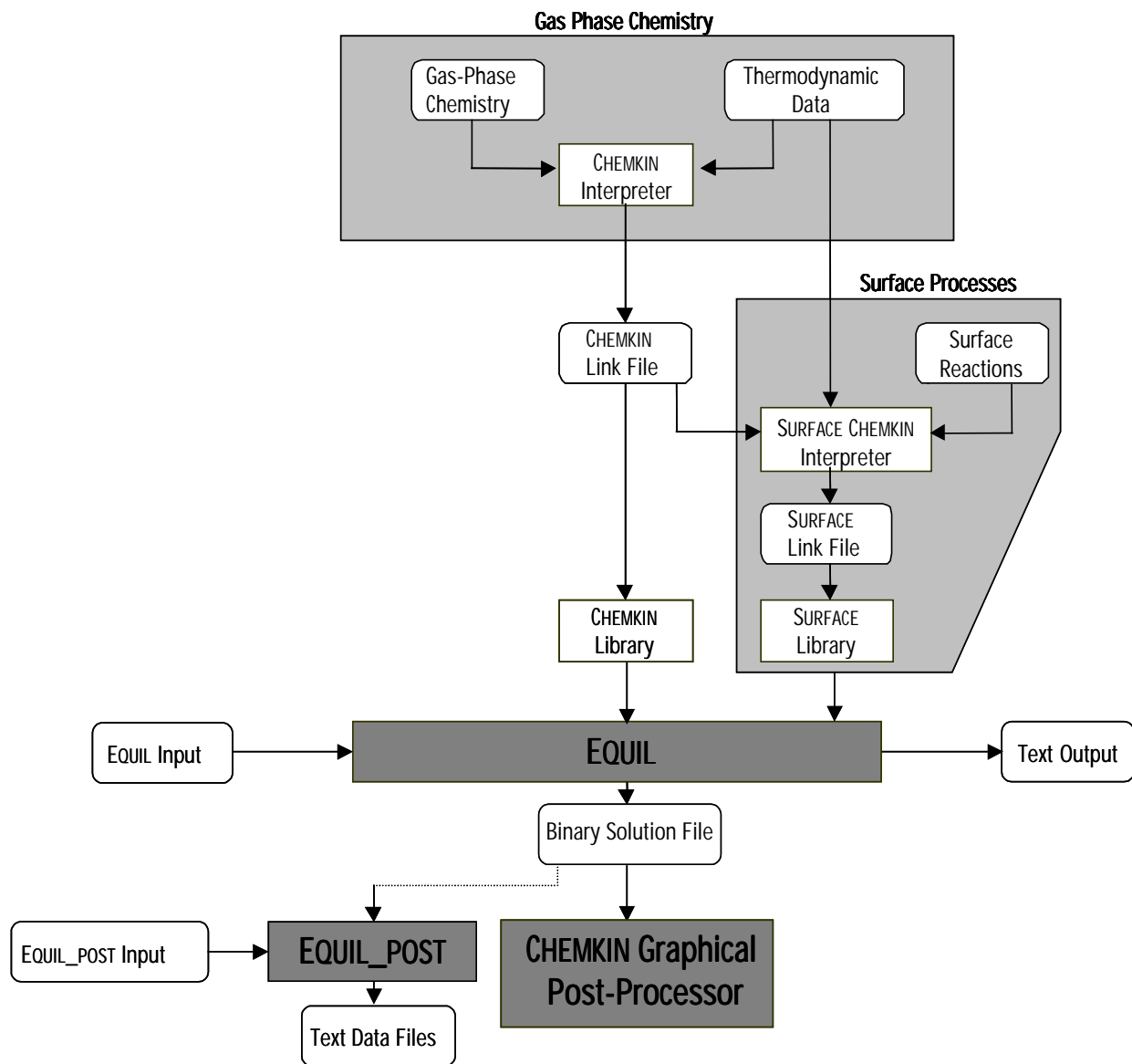

Figure 1.   **Schematic representing the relationship of the EQUIL Application and CHEMKIN.**

3.1 Optional User Programming

In addition to using EQUIL through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to the equilibrium model. To facilitate this, the EQUIL program itself is written as a FORTRAN subroutine that may be called from a user-supplied driver routine. We provide examples of such driver routines as part of the EQUIL software distribution, written in both C++ and FORTRAN. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. EQUIL checks internally to make sure that the allocated work arrays are sufficiently large to address the problem described by the input files. Programs can be linked to the EQUIL subroutine by following the examples in the makefiles provided in the sample driver subdirectories ("drivers_f77" or "drivers_cpp") of the standard distribution. Users taking advantage of this flexibility should be experienced with compiling and linking program files on their operating system and must have either a C++ or Fortran compiler installed.

3.2 The Binary Solution Save File

In addition to printed output the program produces a binary Save File ("save.bin") that contains one or more solutions. More than one solution is included in the case that continuations (Keyword CNTN) were requested. This file is used to post-process the solution. When more than one equilibrium solution is contained on the file, the solutions may be plotted using the CHEMKIN Graphical Post-processor. Further information on this subject can be found in the post-processing discussion in Chapter 5.

4. PROGRAM INPUT

4.1 Keyword Syntax and Rules

The EQUIL program's input is in Keyword format. On each input line, an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. The order of the Keyword inputs is generally unimportant. The rules governing the syntax of the Keyword images are listed below:

1. The first four characters of the line are reserved for the Keyword, and it must begin at the first column.

2. Any further input associated with the Keyword can appear anywhere in columns 5 through 80. The specific starting column is not important.

3. When more than one piece of information is required, the order in which the information appears is important.

4. When numbers are required as input, they may be stated in either integer, floating point, or "E" format. The program converts the numbers to the proper type. The double precision specification is not recognized; however, conversion to double precision is done internally as necessary.

5. When species names are required as input, they must appear exactly as they were specified in the CHEMKIN input. This input is case sensitive.

6. When more than one piece of information is required, the pieces are delimited by one or more blank spaces.

7. If more information is input than required, then the inputs that are read last are used. For example, if the same Keyword is encountered twice, the second one read is taken.

8. A "comment" line can be inserted by placing either a period (.) or a slash (/) in the first column. The program ignores such a line, but it is echoed back in the printed output. In addition, on any Keyword line, any input that follows the required input and is enclosed in parentheses is taken as a comment.

9. The Keyword END must be the last input line.

4.2 Problem Type (Must choose only one)

TP— Constant pressure and temperature conditions.

PT— Constant pressure and temperature conditions.

TV— Constant volume and temperature conditions.

VT— Constant volume and temperature conditions.

TS— Constant entropy and temperature conditions.

ST— Constant entropy and temperature conditions.

PV— Constant pressure and volume conditions.

VP— Constant pressure and volume conditions.

HP— Constant pressure and enthalpy conditions.

PH— Constant pressure and enthalpy conditions.

PS— Constant pressure and entropy conditions.

SP— Constant pressure and entropy conditions.

VU— Constant volume and energy conditions.

UV— Constant volume and energy conditions.

VH— Constant volume and enthalpy conditions.

HV— Constant volume and enthalpy conditions.

VS— Constant volume and entropy conditions.

SV— Constant volume and entropy conditions.

CJ — Chapman-Jouguet detonation. In this case, H, S, V, and T contain the unburned state and TEST gives the burned temperature estimate.

4.3   Constraint Options

FREE — Specifies that the equilibrium composition will be calculated (this is a toggle with the keyword FROZ).

FROZ — Specifies frozen-composition conditions (this is a toggle with the keyword FREE).

FAZE — Specifies a phase constraint on the equilibrium calculation. The gas-phase species are to remain in the gas phase. If there are no bulk species in the mechanism, this constraint has no effect.

CONX — This keyword is used to specify a constant mole fraction for a species.   For example, "CONX H2 0.1" will fix the fraction of hydrogen in the mixture to be 0.1.
    Units — none

4.4   Starting Conditions

TEMP — Specifies the starting temperature for the solution, for example "TEMP 300".
    Units — K

PRES — Specifies the starting pressure for the solution, for example "PRES 1.0".
    Units — atmospheres

VOL — Specifies the starting specific volume for the solution, for example "VOL 198.0 ".
    Units — cm^3/g

ENTH — Specifies the starting enthalpy for the solution, for example "ENTH 1.5E9 ".
    Units — erg/g

ENTR — Specifies the starting entropy for the solution, for example "ENTR 7.0E7 ".
    Units — erg/g-K

ENGY — Specifies the starting energy for the solution, for example "ENGY 1.5E9 ".
    Units — erg/g

REAC — Specifies a reactant mole fraction. A group of these keywords provides the initial composition of the mixture. For example, "REAC O2 0.3" assigns an initial fraction of 0.3 to molecular oxygen, whose CHEMKIN symbol is O2.
    Units — none

4.5   Estimates of Equilibrium Conditions

TEST —   Specifies an estimate of the equilibrium temperature, for example "TEST 2000".
Units — K

PEST —   Specifies an estimate of the equilibrium pressure, for example "PEST 1.1".
Units — atmospheres

4.6   Miscellaneous Keywords

CNTN — Signifies that a continuation set of keywords will follow the END statement. On a continuation, the previous solution is used to provide the initial conditions for the following solution.

END —   This keyword signifies the end of the keywords for a particular EQUIL calculation.

5. POST PROCESSING

5.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from EQUIL. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution date from the "save.bin" file in the working directory. Alternatively, the post-processor may be launched independently and a solution file may be opened from within the Post-processor. The user may open one or more solution files in the Post-processor and may also import external data for comparisons with the simulation results. In addition, the Graphical Post-processor can be used to export all of the solution data into comma-, tab-, or space-delimited text for further analysis with other software packages. For more information on the Graphical Post-processor, please see the CHEMKIN Getting Started manual.

5.2 Configurable Command-line Post-processor

In addition to the CHEMKIN Graphical Post-processor representation of solution data, we provide the user with a FORTRAN post-processor called EQUIL_POST. This program reads the binary solution file and prints selected data to text files, which can then be imported by many other graphics programs. The full source-code, equil_post.f, is provided in the CHEMKIN "post_processors" subdirectory. Also in this directory is a makefile script for re-building the EQUIL_POST program, in case the user makes changes to the source code. In this way, the user may easily configure EQUIL_POST for his or her own analysis needs.

To run EQUIL_POST from the command-line, you will need to do the following:

1. Open a MS-DOS Prompt (PC) or shell (UNIX).

2. Change directories to your working directory, where your "save.bin" solution file resides.

3. Run EQUIL_POST from the command-line, specifying the full path to the CHEMKIN "bin" directory where the "equil_post" executable resides, unless this is already in your environment "path" variable:

```
equil_post < equil_post.inp > equil_post.out
```

Here, "equil_post.inp" is an input file that contains keywords described below. The output "equil_post.out" will contain diagnostics and error messages for the EQUIL_POST run. EQUIL_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of ".csv".

EQUIL_POST uses keyword input. The available keywords are printed as a banner when the program is invoked; they are also described briefly here:

PREF   Requests the text file name be prefixed by a character string.
            Default – "equil"
            Example: PREF equil

SPEC   Requests species fractions for a space-delimited list of species, or "ALL".
            Default - none
            Example: SPEC H2 O2 OH H2O HO2 H O

MOLE   Print species as mole fractions.
            Default - MOLE.

MASS   Print species as mass fractions.
            Default - MOLE.

HELP   Print a brief guide to keyword input.

END   Begin post-processing.

6.   SAMPLE EQUIL PROBLEM A: GAS PHASE EQUILIBRIUM

This sample demonstrates using EQUIL to determine the equilibrium composition for a set of conditions that contain gas-phase species only. The example problem determines equilibrium for a hydrogen/air mixture under adiabatic (constant enthalpy), constant-pressure conditions at one atmosphere. An estimated solution temperature of 2000K is given to ensure that the solution is obtained for an ignited gas. The species that are considered when determining the equilibrium conditions are specified in the CHEMKIN input file "chem.inp".

6.1   Example CHEMKIN Input File

```
ELEMENTS H O N END
SPECIES H2 H O2 O OH HO2 H2O N2 H2O2 END
```

6.2   Example EQUIL Input File

```
REAC H2 2
REAC O2 1
REAC N2 3.76
HP
TEMP 300
TEST 2000
PRES 1
END
```

6.3 Output from EQUIL

```
EQUIL:  Chemkin interface for Stanjan-III
        CHEMKIN-III Version 3.18, 2000/08/14
        DOUBLE PRECISION


                WORKING SPACE REQUIREMENTS
                PROVIDED        REQUIRED
 INTEGER            579              579
 REAL              2052             2052
 CHARACTER           34               34


 CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY,
 DOUBLE PRECISION Vers. 5.28 2000/08/05
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             KEYWORD INPUT

 REAC H2 2
 REAC O2 1
 REAC N2 3.76
 HP
 TEMP 300
 TEST 2000
 PRES 1
 END


  Constant pressure and enthalpy problem.


  EQUIL:  Chemkin interface for Stanjan-III
          CHEMKIN-III Version 3.18, 2000/08/14
          DOUBLE PRECISION

          WORKING SPACE REQUIREMENTS
             PROVIDED        REQUIRED
 INTEGER          485              485
 REAL            1810             1810
 CHAR               9                9
  STANJAN:  Version 3.95, September 1993
            W. C. Reynolds, Stanford Univ.

   MIXTURE:         INITIAL STATE:      EQUILIBRIUM STATE:


 P (atm)              1.0000E+00          1.0000E+00
 T (K)                3.0000E+02          2.3902E+03
 V (cm3/gm)           1.1772E+03          8.0794E+03
 H (erg/gm)           2.6368E+07          2.6368E+07
 U (erg/gm)          -1.1665E+09         -8.1601E+09
 S (erg/gm-K)         8.7862E+07          1.1079E+08
 W (gm/mol)           2.0911E+01          2.4275E+01
 Mol Fractions
 H2                   2.9586E-01          1.4689E-02
 H                    0.0000E+00          1.8294E-03
 O2                   1.4793E-01          5.6253E-03
 O                    0.0000E+00          6.1139E-04
 OH                   0.0000E+00          7.4783E-03
 HO2                  0.0000E+00          1.4207E-06
 H2O                  0.0000E+00          3.2410E-01
 N2                   5.5621E-01          6.4567E-01
 H2O2                 0.0000E+00          1.3816E-07
 Total CPUtime (sec): 0.015625
```

7.   SAMPLE EQUIL PROBLEM B: MULTIPLE PHASE EQUILIBRIUM

This sample demonstrates using EQUIL to determine the equilibrium composition for a set of conditions that include non gas-phase (or "bulk") species. The example problem determines equilibrium for a methane/air mixture under isothermal (constant temperature), constant-pressure conditions at one atmosphere and 300 K. The gas-phase species that are considered when determining the equilibrium conditions are specified in the CHEMKIN input file "chem.inp", while the bulk-phase species are specified in the SURFACE CHEMKIN input file, "surf.inp". In this case the only bulk species included is water.

7.1   Example CHEMKIN Input File

```
ELEMENTS H   O    C   N  AR END
SPECIES
CH4 CO CH3 CH2 CH C H CO2 H2O OH H2O2 HO2 O2 O N2
END
```

7.2   Example SURFACE CHEMKIN Input File

```
BULK/LIQ/
H2O(L) /1./
END
```

7.3   Example EQUIL Input File

```
REAC CH4  1
REAC O2   2.
REAC N2   7.52
TEMP 300
PRES 1
TP
END
```

7.4   Output from EQUIL

```
EQUIL:   Chemkin interface for Stanjan-III
         CHEMKIN-III Version 3.18, 2000/08/14
         DOUBLE PRECISION


                  WORKING SPACE REQUIREMENTS
                  PROVIDED         REQUIRED
INTEGER              1625             1625
REAL                 5785             5785
CHARACTER              83               83


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SKLIB: CHEMKIN-III SURFACE KINETICS LIBRARY,
DOUBLE PRECISION Vers. 7.17 2000/07/02
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          KEYWORD INPUT

REAC CH4  1
REAC O2   2.
REAC N2   7.52
TEMP 300
PRES 1
TP
END


 Constant temperature and pressure problem.

EQUIL:   Chemkin interface for Stanjan-III
         CHEMKIN-III Version 3.18, 2000/08/14
         DOUBLE PRECISION

          WORKING SPACE REQUIREMENTS
                PROVIDED         REQUIRED
INTEGER             1182             1182
REAL                5023             5023
CHAR                  16               16
 STANJAN:  Version 3.95, September 1993
           W. C. Reynolds, Stanford Univ.


 MIXTURE:          INITIAL STATE:      EQUILIBRIUM STATE:

P (atm)               1.0000E+00           1.0000E+00
T (K)                 3.0000E+02           3.0000E+02
V (cm3/gm)            8.9086E+02           7.4766E+02
H (erg/gm)           -2.5561E+09          -3.2712E+10
U (erg/gm)           -3.4588E+09          -3.3470E+10
S (erg/gm-K)          7.2460E+07           6.4313E+07
W (gm/mol)            2.7633E+01           2.7633E+01
Mol Fractions
```

```
CH4                  9.5057E-02          0.0000E+00
CO2                  0.0000E+00          9.5057E-02
H2O                  0.0000E+00          2.9304E-02
O2                   1.9011E-01          1.7668E-31
N2                   7.1483E-01          7.1483E-01
H2O(L)               0.0000E+00          1.6081E-01


   GAS PHASE
Mols                 1.0520E+01          8.8283E+00
W (gm/mol)           2.7633E+01          2.9476E+01
V (cm3/gm)           8.9086E+02          8.3516E+02
Mol Fractions
CH4                  9.5057E-02          0.0000E+00
CO                   0.0000E+00          4.2106E-31
CH3                  0.0000E+00          0.0000E+00
CH2                  0.0000E+00          0.0000E+00
CH                   0.0000E+00          0.0000E+00
C                    0.0000E+00          0.0000E+00
H                    0.0000E+00          0.0000E+00
CO2                  0.0000E+00          1.1327E-01
H2O                  0.0000E+00          3.4919E-02
OH                   0.0000E+00          0.0000E+00
H2O2                 0.0000E+00          0.0000E+00
HO2                  0.0000E+00          0.0000E+00
O2                   1.9011E-01          2.1053E-31
O                    0.0000E+00          0.0000E+00
N2                   7.1483E-01          8.5181E-01


   BULK PHASE: LIQ
Mols                 0.0000E+00          1.6917E+00
Mol Fractions
H2O(L)               0.0000E+00          1.0000E+00
Total CPUtime (sec): 0.015625
```

8. REFERENCES

1. W. C. Reynolds, "The Element Potential Method for Chemical Equilibrium Analysis: Implementation in the Interactive Program STANJAN" Department of Mechanical Engineering, Stanford University (1986).