November 1973 B73-10231

NASA TECH BRIEF

Lewis Research Center

Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems

A computer program has been developed for the calculation of the thermodynamic and transport properties of complex mixtures. The program has the capability of performing calculations such as (1) chemical equilibrium for assigned thermodynamic states, (2) theoretical rocket performance for both equilibrium and frozen compositions during expansion, (3) incident and reflected shock properties, and (4) Chapman-Jouguet detonation properties. Condensed species, as well as gaseous species, are considered in the thermodynamic calculations. However, only gaseous non-ionized species are considered in the transport property calculations.

Many processes in existence today involve complex chemical mixtures, frequently at high temperatures. Some of these mixtures result from combustion processes such as occur in automobiles, aircraft, and rockets. Others occur in processing equipment in the chemical, petroleum, and natural-gas industries. Research equipment, such as shock tubes, also involves high-temperature gas mixtures.

The need frequently arises for the thermodynamic and transport properties of these mixtures, particularly for use in heat- and mass-transfer calculations. Usually, the temperatures of the gases involved are quite high, too high for the properties to be measured directly. Consequently, the properties are calculated. As a result, a number of different computer programs have been written for the property calculations. In general, most of the programs now in existence are designed to calculate either the thermodynamic properties or the transport properties, whereas this program calculates both. The program is a general one, capable of handling any chemical system. Other important features of this program include simplicity of input, storage of all thermodynamic and transport property data on a master tape, and elimination of any need for advance knowledge of which species will be important.

The thermodynamic properties which are tabulated include pressure, temperature, density, enthalpy, entropy, molecular weight $(\partial \ln V/\partial \ln P)_T$, $(\partial \ln V/\partial \ln T)_P$, specific heat at constant pressure, isentropic exponent, sonic velocity, and composition. The calculated transport properties are viscosity, thermal conductivity, and binary and multicomponent diffusion coefficients. Specific heat and thermal conductivity are calculated for both frozen and equilbrium conditions. Prandtl and Lewis numbers are included. Other properties which are characteristic of this type of problem are also calculated.

Transport and relaxation data are provided for 59 species, and additional transport data are provided for interactions between unlike species for another 58 interactions. When transport data are missing for a particular interaction, the data are estimated. The estimating techniques are built into the program. Thermodynamic data for a large number of ideal gases and condensed species are provided with the program for a temperature range of 300 to 5000 K (80 to 8540°F). Transport data are provided over a wider range in many cases. The actual temperature range for each interaction is given in the report in tabular form.

The program input specifies the type of problem to be run, the chemical system of interest, the mixture ratio, and the range of variables. Considerable flexibility is available in specifying the variables. A number of options are available, such as the following:

1. The calculated thermodynamic and transport properties may be obtained on punched cards, as well as printed output.
2. For rocket and shock problems, both equilibrium and frozen properties are available.
3. Input can be specified in a number of different units. For instance, pressure can be given in mm Hg, atmospheres, psia, or newtons/meter^2.
4. Species may be omitted from consideration in the calculations through the use of OMIT cards. Also, certain condensed phases may be included in the initial composition through the use of INSERT cards. Otherwise, only gases are considered initially, which may lead to convergence difficulties.
5. Thermodynamic property calculations can be obtained without including transport property calculations.

The program prints four kinds of output: input data used to do the calculations, information concerning iteration convergence, tables of results, and optional intermediate output.

(continued overleaf)

In order to facilitate adding or deleting applications of the chemical equilibrium part of the program, the program was set up in 10 modules. These modules are concerned with overlay control, general input, additional input processing, four applications, equilibrium calculations, transport calculations, and output.

Notes:

1. Sample problems are given to illustrate some of the features of the program.
2. The program is written in FORTRAN IV for use on an IBM 7094 II/7044 direct couple system or any large computer system.
3. Inquiries concerning this program may be directed to:
   COSMIC
   Information Services
   112 Barrow Hall
   University of Georgia
   Athens, Georgia 30602
   Reference: LEW-11997

Source: R.A. Svehla and B.J. McBride
Lewis Research Center
(LEW-11997)