NASA TECH BRIEF

Computer Program Determines Chemical Equilibria in Complex Systems

The problem:

To solve numerically, nonlinear algebraic equations describing chemical equilibria in complex systems.

The solution:

A computer program for chemical equilibrium computations based on iteration equations that are independent of choice of components.

How it's done:

The NASA Lewis Research Center has developed a computer program for the IBM 7090 or 7094 written in FORTRAN IV for the computation of chemical equilibria in complex systems with several applications. The program permits iteration equations to be written in a form independent of the choice of components. The program can perform the following calculations:

1. chemical equilibrium for assigned temperatures and pressures,
2. theoretical rocket performance for both frozen and equilibrium composition during expansion; and
3. Chapman–Jouguet detonation properties.

The objective has been to develop a program that can compute equilibrium compositions for any chemical system for which thermodynamic data exist. To accomplish this objective, several special techniques were incorporated to handle problems that would otherwise not converge. These techniques, which have proven successful in the many problems attempted, include a flexible convergence control parameter and automatic inclusion of condensed species with the possibility of triple points. A discussion of some of the problems attendant with the presence of condensed species as reaction products is also given.

Notes:

1. The following are some of the program's general features: It requires only a simple input and no initial estimates. It handles up to 15 chemical elements and a total of 90 reaction products including condensed species.
2. The computer program can be used to analyze and study combustion processes and design hardware such as furnaces, combustion engines, chemical reactors, etc.
3. Additional information is contained in NASA Technical Note D-1454, "A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman–Jouguet Detonations," by F. J. Zeleznik and Sanford Gordon, October 1962. Inquiries concerning this innovation may also be directed to:

    Technology Utilization Officer
    Lewis Research Center
    21000 Brookpark Road
    Cleveland, Ohio 44135
    Reference: B66-10671

Patent status:

No patent action is contemplated by NASA.

Source: Frank J. Zeleznik and Sanford Gordon
(Lewis-281)

Category 01