NASA TECH BRIEF

Lewis Research Center

AEROTHERM CHEMICAL EQUILIBRIUM (ACE) COMPUTER PROGRAM

The Problem:

Thermochemical analysis of chemicals in equilibrium.

The Solution:

The Aerotherm Chemical Equilibrium (ACE) computer program is an extremely versatile code for calculating quantities of importance to a broad variety of thermochemical processes.

How It's Done:

The thermochemical processes treated may be divided into two categories: closed systems and open systems. Closed systems are those for which the relative amounts of each chemical element in the system are prespecified. Open systems are those for which the relative amounts of chemical elements depend on various mass transfer rates, due for example, to boundary layer convection or solid surface degradation. The ACE program can treat both systems in chemical equilibrium and systems for which certain reactions are kinetically controlled.

Notes:

1. This program is written in FORTRAN IV for use on an IBM-7094 computer.
2. Inquiries concerning this program should be directed to:

   COSMIC
   Computer Center
   Information Services
   112 Barrow Hall
   University of Georgia
   Athens, Georgia 30601
   Reference: LEW-11722

Source: C.A. Powars and R.M. Kendall
Aerotherm Corporation
under contract to
Lewis Research Center
(LEW-11722)

Category 09