NASA TECH BRIEF

Langley Research Center

Chemical Equilibrium of Ablation Materials Including Condensed Species

The problem:

A method is needed to find the chemical-equilibrium compositions of ablation materials, including condensed species.

The solution:

A computer program has been developed to calculate equilibrium compositions of multiphase systems.

How it's done:

Equilibrium is determined by finding the chemical composition with the minimum free energy. The method of steepest descent is applied to a quadratic representation of the free-energy surface. The solution is initiated by selecting an arbitrary set of mole fractions, from which a point on the free-energy surface is computed.

An n-dimensional parabola (where n equals the number of species) is fitted to the surface at the point corresponding to the initial selection of mole fractions and is oriented in the direction of steepest descent. The minimum of this parabola is obtained by using Lagrangian multipliers to deal with the mass-balance constraints. The coordinates of the minimum, or the point on the parabola closest to the minimum but yielding a set of positive mole fractions, provide a new set of mole fractions from which a new point on the energy surface is calculated.

The procedure is repeated until the change in the set of mole fractions is less than a prescribed value (10^{-5}, for example). The program may be applied to the calculation of chemical-equilibrium compositions of many ablation materials, particularly at temperatures below 2,700 K.

Notes:

1. The program is written entirely in FORTRAN IV, presently for CDC 6000-series machines.
2. Inquiries concerning this program should be directed to:
   COSMIC
   112 Barrow Hall
   University of Georgia
   Athens, Georgia 30601
   Reference: LAR-11801

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