NASA TECH BRIEF

One-Dimensional Reacting Gas Nonequilibrium Performance Program

The problem:

To develop a one-dimensional method for calculating the equilibrium, frozen, and kinetic performance of propellant systems having gaseous exhaust products containing the elements: carbon, hydrogen, oxygen, nitrogen, fluorine, and chlorine.

The solution:

A computer program which calculates the inviscid one-dimensional equilibrium, frozen, and nonequilibrium nozzle expansion of gaseous propellant exhaust mixtures containing the six elements.

How it's done:

The program considers the 19 significant gaseous species present in the exhaust mixtures of propellants containing the above elements and the 48 chemical reactions (13 dissociation–recombination reactions and 35 binary exchange reactions) which can occur between the exhaust products. In order to reduce computation time per case to a minimum, the program uses a second order implicit integration method. This integration method has been demonstrated to reduce the computation time per case several orders of magnitude when directly compared with the computation times required using standard explicit methods such as fourth order Runge–Kutta or Adams–Moulton methods.

The program is completely self-contained, requiring specification of only the propellant system (elemental composition and heat of formation), relaxation rates, and nozzle geometry to run a case. The chemical species considered have been selected to allow accurate equilibrium, frozen, and kinetic performance analyses of cryogenic, space storable, prepackaged, hybrid, and solid propellant systems of current and projected operational use. This program allows analysis of the performance loss associated with film cooling in propellant systems having all gaseous exhaust products. It also allows simultaneous consideration of both chemical and gas-particle relaxation losses in propellant systems having condensed exhaust products. The program is designed for engineering use and is specified and programmed in a straightforward manner to facilitate its use as a development tool.

Notes:

1. The program is written in Fortran IV for use on the IBM 7094 computer.
2. This program will perform calculations for conical nozzles only.
3. Related computer programs are described in NASA Tech Briefs 68-10374, 68-10376, and 68-10377.
4. Inquiries concerning the program may be directed to:

   COSMIC
   Computer Center
   University of Georgia
   Athens, Georgia 30601
   Reference: B68-10375

Patent status:

No patent action is contemplated by NASA.

Source: J. R. Kliegel and H. M. Frey
of TRW Systems
under contract to
Manned Spacecraft Center
(MSC-11777)

Category 06

IS-CAS-42D
RM. 1313 KSC HQS.