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COMPUTER CODES FOR

THERMAL ANALYSIS OF A SOLID ROCKET MOTOR NOZZLE

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ABSTRACT

A number of computer codes are available for performing thermal analysis of solid rocket motor nozzles. Aerotherm Chemical Equilibrium (ACE) computer program can be used to perform one-dimensional gas expansion to determine the state of the gas at each location of a nozzle. The ACE outputs can be used as input to a computer program called Momentum/Energy Integral Technique (MEIT) for predicting boundary layer development, shear and heating on the surface of the nozzle. The output from MEIT can be used as input to another computer program called Aerotherm Charring Material Thermal Response and Ablation Program (CMA). This program is used to calculate ablation or decomposition response of the nozzle material. A new code called Failure Analysis Nonlinear Thermal and Structural Integrated Code (FANTASTIC) is also likely to be used for performing thermal analysis of solid rocket motor nozzles after the program has been duly verified. A part of the verification work on FANTASTIC was done by this author in the summer of 1987 by using one and two-dimension heat transfer examples with known answers. During this summer (1988), an attempt has been made to prepare input for performing thermal analysis of CCT nozzle using FANTASTIC computer code. The CCT nozzle problem will first be solved by using ACE, MEIT, and CMA. The same problem will then be solved using FANTASTIC. These results will then be compared for verification of FANTASTIC.

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INTRODUCTION

Failure Analysis Associates (FAA), Palo Alto, California has developed an advanced computer code for MSFC to improve the accuracy of the solid rocket nozzle motor analysis. The computer code is called "FANTASTIC", an acronym for Failure Analysis Nonlinear Thermal And Structural Integrated Code. This code incorporates a higher order integration scheme for modeling steep temperature and strain gradients. It has a modular design and is intended as a multi-purpose thermostructural analysis code.

The first version of the above code was released by FAA in the beginning of 1987. This author worked as NASA/ASEE Summer Faculty Fellow at MSFC in the summer of 1987 and got an opportunity to study and verify this code. A number of one and two-dimensional heat transfer problems were developed and run on FANTASTIC for trial. The problems faced during these trial runs were reported to the developer. As a result, the code was improved and a second revised version of the program was released which could solve simple problems.

In the summer of 1988, the author returned to MSFC as a Summer Faculty Fellow and started working on FANTASTIC but with a different approach. The aim was to verify FANTASTIC for the analysis of solid rocket motor nozzles (SRM). This prompted the author to design a problem which could be first solved using existing codes with MSFC.

CCT-5 nozzle was selected as an example. The author studied one existing code called Aerotherm Chemical Equilibrium (ACE) computer program. Other codes which will be needed to make a complete thermal analysis for CCT-5 nozzle are called Momentum/Energy Integral Technique (MEIT) and Aerotherm Charing Material Thermal Response and Ablation Program (CMA). A brief review of running ACE and pertinent information about these codes is given in the next section.

ACE COMPUTER PROGRAM

ACE program was developed by Acurex Corporation, Mountain View, California for MSFC. It is an extremely versatile code for calculations of a number of thermochemical processes taking place in closed or open system. A few types of calculations which may be performed by ACE are:

1. The thermodynamic and chemical state in the combustion chamber of the SRM may be calculated by specifying the elemental composition of the injected fuel.

2. ACE can perform an isentropic expansion of the combustion gases and boundary layer edge state tables may be calculated for subsequent input to heat conduction and ablation energy balance programs.

3. The thermodynamic state at the surface of an ablation material may be calculated as a function of pyrolysis gas and char rates normalized with respect to mass transfer coefficients.

Combustion Chamber Gas Expansion Calculation Using ACE

The input data card deck for running ACE may consist of the following seven card sets:

1. Control card
2. Surface fluxes
3. Oblique or normal shock data
4. Elemental composition data
5. Fuel temperature and diffusion factor data
6. Species thermochemical equilibrium data
7. Reaction rate data

Card set 1 is a control card which contains a 10 element array, KR(I). This array controls most of the program options and tells the program what to expect from the remaining card sets. Few problems require all card sets.

As an example the input for performing combustion chamber calculation and further gas expansion for a range of pressure values is given below:

Card Set 1

Control Card (1 Card)

Field 1

(Column 1-10) this is the variable array KR(I) which is used to control the various program options

Column 1: State Option

0 for "Assigned temperature"

Column 2: Elemental Composition

1 for "Input new elemental compositions" in card set 4.

Column 3: Species thermochemical data

1 for "Read from cards new species thermochemistry data (card set 6) and, if provided, data on fail temperatures and diffusion factors (card set 5)

Column 4: Mass balance options

0 for "Closed system mass balance"

Column 5: Expansion Option

2 for "Save the current enthalpy as a chamber enthalpy, and save the current entropy, for subsequent isentropic expansion calculations.

Columns 6 through 10 "0"

Field 2

(Columns 11-20) The thermodynamic state variable Y since in column 1 of Field 1, KR(1) = 0, therefore, Y is assigned to temperature (^ok).

(Y = 3430.0 for this example)

Field 3

(Columns 21-30) Pressure variable, PR
If PR 0, PR is assigned to the system pressure in atmospheres.
(PR = 68.0735 for this example).

Field 4 - Field 6

(Columns 31-80)
No input needed for this example

Card Sets 2-3

No input needed

Card Set 4

Card 1

(Columns 1-3) The number of elements in the system

Cards 2, 3, 4,....(one such card for each element)

Field 1

(Columns 1-3) the atomic number of the element

Field 2

(Columns 4-15) the name of the element

Field 3

(Columns 16-25) the atomic weight of the element

Field 4

(Columns 26-55) the relative amounts of the element in components
1, 2, and 3, respectively.

The input for the current example for Card Set 4 is given below:

COLUMNS

	<u>(1-3)</u>	<u>(4-15)</u>	<u>(16-25)</u>	<u>(26-55)</u>
Card 1	6			
Card 2	1	Hydrogen	1.008	3.7176
CARD 3	6	Carbon	12.011	0.9407
Card 4	7	Nitrogen	14.011	0.6263
Card 5	8	Oxygen	16.000	2.4396
Card 6	13	Aluminum	26.982	0.5930
Card 7	17	Chlorine	35.457	0.5952

CARD SET 6

SPECIES THERMOCHEMICAL EQUILIBRIUM DATA

(Number of cards = 1 + 3 x number of species) see note

If KR(3) = 0,5,6,7,8 or 9, skip this card set

There are three of these cards for each molecular, atomic, condensed, ionic, or electron species. The end of this card set is signaled by a blank card (see Reference 3 for additional discussion relative to this card set)

CARDS 1,4,7 . . . Describe the elemental composition of the species and establish its name designation

FIELDS 1,3,5, . . . ,13. (one for each element in the species)

(Columns 1-3, 7-9, 13-15, . . . ,37-39, each format F3.0)

The number of atoms (of atomic number given in the following field) in a molecule of this species

(If field 1 is zero, this card is presumed to represent the end of Card Set 6)

FIELDS 2,4,6, . . . ,14 (one for each element in the species)

(Columns 4-6,10-12,16-18, . . . ,40-42, each format I3)

The atomic numbers of the elements in the molecule (the number of atoms of which was given in the previous field)

(If field 2 is zero, this card is presumed to be the first card of Card Set 5)

Ionized species are described by the addition or subtraction of an electron (atomic number 99). For example, NO^+ would be described in fields 1 through 6 as bb1bb7bb1bb8b-1b99.

FIELD 15

(Columns 43-72, Format 7A4A2) the source and date of the thermochemical data for this specie. Used for output only

FIELD 16

(Columns 73-80, Format 2A4) the name designation of this species (e.g., AL203). This variable is used for output and as a means of identifying data entered in Card Set 5

FIELD 16 (Continued)

NOTE: The ACE code is dimensioned such that the number of chemical species may not exceed 149. Also the number of condensed phase species may not exceed (14-number of elements).

CARDS 2,5,8...Lower temperature range thermochemical data

FIELDS 1,2,3,4,5 and 6

(Columns 1-54, Format 6E9.6) Input the 6 constants (F1,F2,F3,F4,F5,F6) appropriate to the lower temperature range of the thermodynamic data for this species. These constants are defined as follows, where T is in OK:

F1 = the heat of formation of the species at 298OK from the JANAF base state (elements in most natural form at 298OK) in cal/mole

F2 = the enthalpy change of the species from 298OK to 3000OK in cal/mole

F3,F4 and F5 are defined by a curve fit to the heat capacity at constant pressure of the form:

$$C_p = F3 + F4 T + \frac{F5}{T^2} \text{ in cal/mole } ^\circ\text{K}$$

F6 = the entropy of the species at 3000OK in cal/mole OK

FIELD 7

(Columns 61-66, Format F6.0) the upper limit of the lower temperature range in OK

FIELD 8

(Column 67, Format II) the phase specification:

- 1 signifies gaseous species
- 2 signifies solid species
- 3 signifies liquid species

The only phase combination allowed in one three card set is solid-liquid in which case a 2 and 3 would appear in fields 8 of cards 2 and 3, respectively.

CARDS 3,6,9...Upper temperature range thermochemical data

These cards are the same as cards 2,5,8...except use constants for the upper temperature range and field 7 is ignored

LAST CARD OF CARD SET 6 MUST BE BLANK

OVERALL PROCEDURE OUTLINE AND CONCLUSIONS

An outline of the procedure to be following for analysing the SRM nozzle problem using different computer codes is as follows:

1. Preparation of input for ACE
2. Run ACE expansion
3. To arrange the output from ACE in an acceptable format for running MEIT
4. Run MEIT for boundary layer analysis
5. Preparation of ablation tables using output from MEIT. The ablation tables are used as input for CMA
6. Run CMA
7. Work on input for FANTASTIC
8. Run FANTASTIC
9. Compare the results from CMA with those from FANTASTIC

The first three steps have been completed. The work on last the last three steps can be started after FANTASTIC has been revised for handling nozzle problem. The work on steps 4-6 can be continued.