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AEROTHERM FINAL REPORT NO. 67-13

(Computer Program Writeup)

May 4, 1967

THE NON-NEUTRAL IONIZED CHEMICAL EQUILIBRIUM SUBROUTINE

by

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Prepared for

National Aeronautics and Space Administration
Ames Research Center
Moffett Field, California 94305

Contract NAS2-3929

Aerotherm Project No. 6025

THE NON-NEUTRAL IONIZED CHEMICAL EQUILIBRIUM SUBROUTINE

SECTION 1
INTRODUCTION

The Non-neutral Ionized Chemical Equilibrium Subroutine was prepared for utilization with a general viscous shock layer program being developed at the Ames Research Center of NASA. It serves to isolate the complexities of the chemistry solution outside of the logic associated with the shock layer solution and thus to permit greater flexibility of operation. The NICHE subroutine treats a general chemical system composed of up to 25 arbitrarily selected molecules and ions. It evaluates the state based on assigned elemental composition, surplus or deficit of charge, pressure and enthalpy (or temperature). The state evaluation yields composition, temperature (or enthalpy), and derivatives of these properties with respect to the input parameters.

To accelerate its operation when coupled to the viscous shock layer, certain special features have been included in this subroutine. These include 1) separation of the input features into a separate main program which prepares a binary data tape, and 2) optimization of first guesses by storing the variables necessary to specify these guesses at each shock layer station.

In addition to the thermodynamic state specification, certain terms appropriate to transport property evaluation are determined. These terms are described in Reference 1.

This report describes the operation of the subroutine including the preparation of input, the communication between it and the calling routine, the general nature of the solution process and the accuracy of the calculated derivatives.

SECTION 2
PROGRAM INPUT

A separate program (INPUT) is used to read all the necessary input data required by the NICHE subroutine. This data is manipulated and organized and placed on a binary tape for subsequent use by the NICHE subroutine.

The input to INPUT is of three types - elemental information, diffusion factor data, and thermodynamic data. The form and nature of this input is described in the following paragraphs.

ELEMENTAL DATA

Card 1, Format 2I3, F11.4

Field 1 (Cols. 1-3, right justified)

Number of elements in the system (in ionized systems the electron is treated as an additional element).

Field 2 (Cols. 4-6, right justified)

Logical unit number on which binary output from the program will be stored.

Field 3 (Cols. 7-17)

Power on molecular weight if assumption that $F_i \propto \mathcal{M}_i$ to a power is used. Power presumed to be 0.5 if no entry is provided. The F_i (see Ref. 1) are referenced to $\overline{D}$ which approximates, in this case, the self-diffusion coefficient of O_2, specifically,

$$\overline{D} = 4.168 \times 10^{-8} \, T^{3/2}/(P\Omega)$$

$$\Omega = 1.07(T/106.7)^{.159}$$

where $\overline{D}$ is ft^2/sec, T is in ^oK and P is in atmospheres. The constant in the first equation presumes a collision radius of 3.467 $\mathring{A}$. The latter equation is based on a curve fit of Leonard-Jones cross-sections as a function of reduced temperatures with ϵ/k for O_2 taken as 106.7.

Cards 2, 3, ..., one for each element, Format I3, 3A4, F10.5

Field 1 (Cols. 1-3, right justified)

Atomic number of element (99 for electron). Cards are ordered with this number ascending.

Field 2 (Cols. 4-15)

Name of element (for output only)

Field 3 (Cols. 16-25)

Atomic weight of element.

DIFFUSION FACTOR DATA

Card 1, Format I3

Field 1 (Cols. 1-3, right justified)

Negative number of molecules for which diffusion factor data is being supplied. Other molecules will use power on molecular weight approximation:

$$F_i = \left(\frac{m_i}{28}\right) \text{ to power}$$

If value is positive this card is assumed to be first card of next set (thermodynamic data)

Card 2, ..., if and as required, Format 4(2A4, E12.4)

Field 1, 3, 5, and 7 (Cols. 1-8, 21-28, 41-48 and 61-68)
Name of molecule as it appears in Cols. 73-80 on first card of 3-card thermodynamic data set for the molecule.

Field 2, 4, 6 and 8 (Cols. 9-20, 29-40, 49-60 and 69-80)
Diffusion factor F_i for molecule

THERMODYNAMIC DATA

(3 cards for each molecule, blank card after last molecular set concludes thermodynamic data.)

Card 1, 4, 7, ..., Format (7(F3.0, I3), 30X A6A2)

Field 1, 3, 5, ..., one for each element in molecule (Cols. 1-3, 7-9, 13-15,...)
Number of atoms (of atomic number given in subsequent field) in a molecule of this species. If field one is negative this card is presumed to be first card of diffusion factor data set. If field one is zero this card is presumed to be end of thermodynamic data.

Field 2, 4, 6, ..., one for each element in molecule (Cols. 4-6, 10-12, 16-18, ...)
Atomic number of elements in molecules listed in ascending sequence.

Last Field (Cols. 73-80)
Molecular designation for output and as identifier for diffusion factor data.

Card 2, 5, 8, ..., one for each molecule (Format 6E9.6,6X, F6.0, I1

Field 1 (Cols. 1-9)
Heat of formation of molecule at 298°K from JANAF base state (elements in most natural form at 298°K) cal/mole.

Fields 2-6 (Cols. 10-18, 19-27, 28-36, 37-45 and 46-54)
Constants appropriate to lower temperature range of thermodynamic data (see below)

Field 7 (Cols. 61-66)
Upper limit of lower temperature range in °K.

Field 8 (Col. 67)

Zero indicates gaseous species.

Taking F_2, F_3, ..., as Fields 2, 3, etc., the curve fits are as follows:

$$C_p = F_3 + F_4T + F_5/T^2$$

$$h - h_{298} = F_2 + \left[F_3T + \frac{1}{2} F_4T^2 - F_5/T\right]_{3000}^{T}$$

$$s = F_6 + \left[F_3 \ln T + F_4T - \frac{1}{2} F_4T - \frac{1}{2} F_5/T^2\right]_{3000}^{T}$$

with T in °K h in cal/mole and s in cal/mole °K

Card 3, 6, 9, ..., one for each molecule, Format 6E9.6, 6X, F6.0, I1

Same as Cards 2, 5, 8 except for upper temperature range and Field 7 is ignored.

The arrangement of these card sets is of consequence in so far as it determines the "elemental" order of the system of mass balance equations, a significant factor in the communication between the shock layer and chemistry routines. If the first five molecules are O_2, C, H_2, N_2, e^-, then the mass balance indices must correspond with oxygen as one, carbon as 2, etc., with the charge balance occurring as the fifth balance. For a general discussion of the term "element" as used by these routines, see Reference 2.

The tape that is prepared by the INPUT program will subsequently be read by the Subroutine EQUIL on the first call from the shock layer routine. This represents the extent of outside input to the NICHE subroutine. Additional information is provided to it via the call from the shock layer routine and through COMMON. This communication will be discussed in the next section.

SECTION 3
COMMUNICATION WITH CALLING ROUTINE

The call list provides communication for temperature (or enthalpy) and pressure, in that order. All other variables are communicated via COMMON. COMMON/ACEC/ is the principal vehicle for this communication, although certain variables are also communicated via COMMON/EQUI/and/MAINC/. The following table serves to identify these variables, as well as those in the call list.

CALL EQUIL LIST

Z	enthalpy in cal/gm, if IU = NPU temperature in ^{o}K, if IU $\neq$ NPU dummy if Z = 0
PRR	pressure in atm if PRR $\neq$ 0
COMMON/ACEC/*	(all variables generated in NICHE)
VNU(j,i)	stoichiometric coefficients in formation of one molecule of j from base species i. The base species are the first IS molecules in the thermodynamic data set where IS is the number of elements. This set will be rearranged by the INPUT program, if necessary, to achieve a valid set of base species.
CI(j)	mass fraction of molecule j
DIT(j)	multicomponent thermal diffusion coefficient of molecule j. See Reference 1.
DVDCP(j,i)	derivative of mole fraction of molecule j with respect to mass fraction of "element" i at constant temperature and pressure, times molecular weight of "element" i
DVDP(j)	derivative of mole fraction fo molecule j with respect to pressure (in atmospheres) at constant temperature and "elemental" mass fractions
DVDT(j)	derivative of mole fraction of molecule j with respect to temperature (in ^{o}K) at constant pressure and "elemental" mass fractions
FF(j)	diffusion factor F of molecule j
H(j)	enthalpy of molecule j in cal/gm
FAMOA(j)	first six characters in designation of molecule j
VN(j)	mole fraction of molecule j
WTM(j)	molecular weight of molecule j. Note that the first IS members of this array are the molecular weights of the "elements"
ZI(j)	diffusive mass fraction of molecule j (see Ref. 1) also referred to as Z-potential
CPF	frozen heat capacity of system in cal/gm^{o}K
DBAR	$\overline{D}$ of Reference 1 in ft^{2}/sec. See discussion in preceding section
HIP	enthalpy of system in cal/gm

*This entire common as well as COMMON/ACRE/ are equivalenced to ACECE and ACREE in order to facilitate storage and retrieval from the binary tape.

P	pressure in atmospheres
RHO	density of system in lb/ft^3
T	system temperature in ^oK
VLAM	thermal conductivity of system in Btu/ft ^oR
VMU	viscosity of system in lb/ft sec
VMU1	μ_1 of Reference 1
VMU2	μ_2 of Reference 1
WM	system molecular weight
COMMON/EQUI/	(all variables unaltered by NICHE)
CPPS(i)	mass fraction of "element" i divided by molecular weight of "element" i at the edge of the shock layer. Used to define "elemental" composition of system if IU = NPU
COMMON/MAINC/	(all variables unaltered by NICHE)
CIA(ℓ,j)	mass fraction of molecule j at station ℓ in shock layer. Used to define initial guesses in NICHE after calculations have once been performed at station ℓ
CPP(ℓ,j)	mass fraction of "element" i divided by molecular weight of "element" i at station ℓ in shock layer. Used to define "elemental" composition of system if IU $\neq$ NPU
I9(1)	logical unit number from which binary information generated by INPUT is to be read on first entry into EQUIL
I9(2)	on first call of EQUIL used to establish KR(9). Subsequently KR(9) = 0 yield full unequal diffusion and thermal diffusion model, KR(9) = 1 eliminates thermal diffusion and KR(9) = 2 yields equal diffusion coefficients with no thermal diffusion
IU	index ℓ on shock layer surface normal coordinate. (= 1 at wall, = NPU at shock wave)
IY	on first call of EQUIL used to establish debug output flag KR(7) namely KR(7) = 5*IY - 4. If KR(7) > 1 full debug output is printed at each iteration and KR(7) is decremented by 1. If KR(7) > 0 single line of debug output is printed at each iteration. KR(7) is <u>not</u> reinitialized with each call.
NPU	number of stations in surface normal direction
COMMON/ACRE/	(not used outside of Niche but...)
VMW(ℓ)	molecular weight at station ℓ in shock layer. Used to establish initial guesses after first entry into EQUIL at station ℓ
IFFI(ℓ)	flag used to establish if prior entry at station ℓ has occurred.

The dimensions on variables are consistent with the subscripts given above. As currently compiled the limits on the indices are

j	25
i	6
ℓ	11

Variables dimensioned 25 or 26 are related to j. Variables dimensioned 6, 7 or 10 (except KR(10)) are related to i. All other variables in NICHE have fixed dimensions, except ACECE and ACREE which are dimensioned to contain all of COMMON/ACEC/ and COMMON/ACRE/, respectively.

SECTION 4
GENERAL NATURE OF SOLUTION

In Reference 2 a general description of the solution procedure is presented. Certain specific aspects of the solution process with regard to non-neutral chemical states deserves discussion here, however. The charge balance is treated together with the elemental mass balances by a relation of the form

$$\sum p_j \nu_{j,i} = \rho \mathcal{M} \alpha_i$$

where i is the index appropriate to the mass or charge balance, the p_j are partial pressures of molecule j in the system, the ν_{ji} are the stoichiometric coefficients in the formation of one molecule of j from the base species, $\mathcal{M}$ is the system molecular weight and α_i is the conserved variable associated with "elemental" mass balances or the charge balance. In the charge balance (i = e) with the electron taken as the only charged base species, $\nu_{j,e}$ represents the negative charge on molecule j. For example, $\nu_{j,e}$ for NO^+ and O_2^- are -1 and +1, respectively. For a neutral system α_e is zero. If there is a charge deficit $\alpha_e < 0$ yielding a net positive charge on the system. Specifically α_e is the charge excess in a one gram system divided by Avogadro's number.

The transport property model of Reference 1 is, by implication, being applied to ionized systems. The wisdom of this application is open to serious question in highly ionized systems. For neutral slightly ionized systems, the model is probably useful and certainly will indicate, under more severe conditions, major trends in the non-neutral ionized shock layer.

SECTION 5
DERIVATIVE CALCULATIONS

The evaluation of various partial derivatives is a major aspect of the solution procedure. In order to demonstrate the accuracy of this procedure Tables I(a)-I(f) were prepared. These tables indicate the state solution at the mass fractions, temperature and pressure given in Table I(a) and at a set of incrementally different states, with only one parameter being incremented for each solution. Thus the indicated derivatives can be checked. The checks yielded uniformly accurate results. For example

$$\frac{\partial p_{e^-}}{\partial T} = 1.406 \times 10^{-5} \text{ and } 1.294 \times 10^{-5} \qquad \text{Tables I(a) and I(f)}$$

$$= 1.350 \times 10^{-5}$$

By finite difference I(a) less I(f)

$$\frac{\partial p_{e^-}}{\partial T} = \frac{2.2436 \times 10^{-2} - 2.1086 \times 10^{-2}}{9000 - 8900} = 1.350 \times 10^{-5}$$

Or, letting $\tilde{K}_c$ represent the mass fraction of the element carbon,

$$\frac{\partial p_{c^+}}{\partial \tilde{K}_c} = 3.672 \times 10^{-2} \text{ and } 3.797 \times 10^{-2} \qquad \text{Tables I(a) and I(b)}$$

$$= 3.734 \times 10^{-2}$$

and by finite difference I(a) less I(b)

$$\frac{\partial p_{c^+}}{\partial \tilde{K}_c} = \frac{9.6200 \times 10^{-3} - 9.2467 \times 10^{-3}}{1.753 \times 10^{-1} - 1.653 \times 10^{-1}} = 3.733 \times 10^{-2}$$

SECTION 6
RECOMMENDATIONS

Because of the uncertainties of the transport property model of Reference 1 as applied to highly ionized non-neutral systems, it is recommended that "exact" first order transport property relations be used to evaluate fluxes in the shock layer solution. This would involve inclusion of cross-section data for each diffusing pair. Inasmuch as a single potential model is inappropriate for all pairs in an ionized system, input preparation would become more extensive but uncertainties would be better defined. It appears that the inclusion of this model would not necessitate any major modification of the shock layer program.

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(a) Base State

				DERIVITIVES OF MOLE FR.WITH RESPECT TO--						
				TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$	$\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
NAME	MOLE FR	MASS FR	Z POT. 9.0[illegible]E	[illegible] 1.	E [illegible]	1.753E- 1	5.5[illegible]E- 7	2.[illegible]2 E-[illegible]2	5.9 8E-[illegible]1	2.138E-.1
C	1.4798E-01	1.6292E-01	1.6742E-01	-1.226E-05	6.591E- 3	7.142E-01	3.262E [illegible]3	-1.[illegible]73E 00	-1.181E-.1	-1.[illegible]95E-01
E-	2.2436E-02	1.1312E-06	1.7177E-04	1.4[illegible]6E-05	-7.236E- 3	2.265E-02	1.313E [illegible]4	-1.646E-01	-9.9[illegible]3E-[illegible]3	-9.41[illegible]E-[illegible]3
H	2.1873E-01	2.[illegible]199E- 2	7.1662E-[illegible]2	-5.235E-[illegible]6	2.964E- 3	-2.[illegible]75E-01	-2.938E [illegible]3	8.426E 00	-1.696E-01	-1.[illegible]0E-01
N	4.4913E-01	5.7672E-01	5.4876E-01	4.151E-[illegible]7	-1.966E- 3	-4.179E-01	-5.[illegible]54E [illegible]3	-4.841E [illegible]0	4. [illegible]8E-[illegible]1	-3.[illegible]29E- 1
O	1.44[illegible]5E-01	2.1127E-01	1.8910E-01	-1.735E-06	8.176E-[illegible]4	-1.42[illegible]E-01	-1.758E [illegible]3	-1.[illegible]69E 00	-1.1[illegible]E-01	5.759E-01
C2	1.7885E-05	3.9333E-05	2.8616E-05	-1.958[illegible]E-08	1.948E-[illegible]5	1.726E-04	7.885E-01	-4.[illegible]45E-04	-2.654E-[illegible]5	-2.648E-05
H2	8.1[illegible]98E-06	1.4979E-[illegible]6	3.7581E-[illegible]6	-5.98[illegible]E-[illegible]9	8.33 E- 6	-1.[illegible]39E-05	-2.179E-01	6.249E-04	-1.2[illegible]7E-[illegible]5	-1.112E-05
N2	4.4687E-03	1.1476E-[illegible]2	7.7215E-03	-6.816E-[illegible]6	4.43 E- 3	-8.316E-[illegible]3	-1.[illegible]6E [illegible]2	-9.[illegible]34E-[illegible]2	8.[illegible]36E-[illegible]3	-6.[illegible]28E-03
O2	1.7758E-[illegible]6	5.2 9 E-06	3.2794E-06	-1.371E-09	1.796E-[illegible]6	-3.502E-06	-4.333E-[illegible]2	-3.868E-05	-2.736E-06	1.42[illegible]E-05
C+	9.62[illegible]E-[illegible]3	1.[illegible]591E-[illegible]2	1.[illegible]884E-[illegible]2	1.1[illegible]3E-[illegible]5	-6.[illegible]89E- 3	3.672E-02	-5.418E [illegible]3	-3.[illegible]23E-02	-3.425E-[illegible]3	-3.[illegible]86E-03
N+	1.5553E-[illegible]3	1.997 E-[illegible]3	1.99[illegible]3E-[illegible]3	2.677E-[illegible]6	-1.[illegible]6[illegible]E- 3	-3.[illegible]17E-[illegible]3	-9.278E [illegible]2	-5.357E-03	2.[illegible]86E-[illegible]3	-3.966E-04
O+	3.5160E-04	5.1566E-[illegible]4	4.5912E-04	5.656E-[illegible]7	-2.362E- 4	-7.[illegible]17E-[illegible]4	-2.1 1E [illegible]2	-1.251E-[illegible]3	-1.1[illegible]5E-[illegible]4	1.553E-[illegible]3
CHN	2.7496E-[illegible]8	6.8119E-[illegible]8	4.6654E-[illegible]8	-5.723E-11	5.647E-[illegible]8	8.[illegible]03E-[illegible]8	-7.268E-05	4.[illegible]20E-07	-1.853E-[illegible]6	-5.776E-08
CN	3.3415E-04	7.9696E-[illegible]4	5.5642E-04	-3.98[illegible]E-07	3.476E-[illegible]4	1.[illegible]02E-03	3.6[illegible]6E [illegible]0	-7.381E-[illegible]3	3.[illegible]36E-[illegible]5	-4.727E-04
CO	1.2262E-[illegible]3	3.1484E-[illegible]3	2.1185E-[illegible]3	-2.2[illegible]9E-06	1.288E- 3	4.7[illegible]9E-03	1.2[illegible]7E [illegible]1	-2.722E-02	-1.923E-[illegible]3	3.994E-03
NO	1.1006E-04	3.[illegible]276E-04	1.9683E-[illegible]4	-1.135E-[illegible]7	1.1[illegible]2E- 4	-2.11[illegible]E-[illegible]4	-2.581E [illegible]1	-2.[illegible]85E-[illegible]3	1.418E-[illegible]5	3.658E-04
C2H	2.9591E-[illegible]9	6.7893E-[illegible]9	4.8329E-09	-5.921E-12	6.[illegible]22E-[illegible]9	2.576E-08	9.071E-[illegible]5	4.708E-08	-7.[illegible]16E-[illegible]9	-6.41[illegible]E-[illegible]9
C3H	1.[illegible]785E-13	3.6618E-[illegible]3	2.1427E-13	-3.3[illegible]9E-16	3.394E-13	1.459E-12	5.683E-[illegible]9	4.962E-13	-3.417E-[illegible]3	-3.135E-13
C4H	2.1967E-17	9.886 E-17	5.[illegible]27[illegible]E-17	-8.835E-[illegible]9	9.21[illegible]E-17	4.[illegible]36E-16	1.643E-12	-1.475E-16	-8.721E-17	-8.[illegible]18E-17
C2H2	5.9854E-14	1.4285E-13	9.97[illegible]2E-14	-1.6[illegible]E-16	1.865E-13	4.642E-13	1.[illegible]31E-[illegible]9	3.258E-12	-1.[illegible]83E-13	-1.7[illegible]7E-13
HO	9.8[illegible]6[illegible]E-[illegible]6	1.5288E-05	1.32[illegible]2E-05	-7.324E-09	9.995E-[illegible]6	-1.897E-[illegible]5	-2.514E-[illegible]1	2.710E-04	-1.516E-[illegible]5	3.248E-05
C3	2.6878E-[illegible]7	9.8779E-[illegible]7	5.2671E-[illegible]7	-6.374E-13	5.735E-[illegible]8	3.[illegible]92E-[illegible]9	1.778E-[illegible]5	-9.[illegible]19E-[illegible]9	-6.433E-[illegible]8	-5.969E-[illegible]7

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(b) Decremented Carbon Mass Fraction

			DERIVITIVES OF MOLE FR.WITH RESPECT TO --						
			TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$	$\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
NAME	MOLE FR	MASS FR	Z POT. 9.0[illegible]E 03	1.0[illegible]E 00	1.653E-01	5.500E-07	2.020E-02	5.908E-01	2.138E-01
C	1.4077E-01	1.5352E-01	1.5939E-01	-1.176E-05	6.329E-03	7.272E-01	3.255E-03	-1.678E-00	-1.134E-01
E-	2.2205E-02	1.1089E-06	1.7014E-04	1.377E-05	-7.069E-03	2.351E-02	1.334E-04	-1.654E-01	-9.928E-03
H	2.2080E-01	2.0198E-02	7.2474E-02	-5.223E-06	2.958E-03	-2.115E-01	-3.913E-03	8.484E-00	-1.728E-01
N	4.5335E-01	5.7661E-01	5.5434E-01	6.116E-07	-2.100E-03	-4.259E-01	-5.162E-03	-4.932E-00	4.043E-01
O	1.4549E-01	2.1135E-01	1.9012E-01	-1.823E-06	8.675E-04	-1.449E-01	-1.798E-03	-1.602E-00	-1.132E-01
C2	1.6186E-05	3.5332E-05	2.5917E-05	-1.774E-08	1.764E-05	1.672E-04	7.486E-01	-3.697E-04	-2.608E-05
H2	8.2659E-06	1.5123E-06	3.8334E-06	-6.091E-09	8.487E-06	-1.584E-05	-2.256E-01	6.352E-04	-1.294E-05
N2	4.5532E-03	1.1582E-02	7.8737E-03	-6.941E-06	4.511E-03	-8.555E-03	-1.037E-02	-9.908E-02	8.122E-03
O2	1.8114E-06	5.2629E-06	3.3476E-06	-1.400E-09	1.833E-06	-3.609E-06	-4.477E-02	-3.985E-05	-2.818E-06
C+	9.2467E-03	1.0084E-02	1.0469E-02	1.071E-05	-5.837E-03	3.797E-02	-5.342E-03	-3.672E-02	-3.314E-03
N+	1.5862E-03	2.0174E-03	1.9396E-03	2.741E-06	-1.089E-03	-3.179E-03	-9.711E-02	-5.446E-03	2.124E-03
O+	3.5879E-04	5.2122E-04	4.6887E-04	5.794E-07	-2.424E-04	-7.374E-04	-2.200E-02	-1.273E-03	-1.187E-04
CHN	2.6656E-08	6.5411E-08	4.5273E-08	-5.548E-11	5.474E-08	8.712E-08	-5.091E-05	4.298E-07	-1.856E-08
CN	3.2086E-04	7.5800E-04	5.3470E-04	-3.823E-07	3.338E-04	1.356E-03	3.766E-00	-7.156E-03	2.770E-05
CO	1.1781E-03	2.9962E-03	2.0370E-03	-2.123E-06	1.238E-03	4.912E-03	1.268E-01	-2.641E-02	-1.865E-03
NO	1.1221E-04	3.0572E-04	2.0081E-04	-1.157E-07	1.124E-04	-2.172E-04	-2.664E-00	-2.455E-03	1.279E-05
C2H	2.7036E-09	6.1441E-09	4.4190E-09	-5.413E-12	5.686E-09	2.534E-08	8.814E-05	4.212E-08	-6.471E-09
C3H	9.3735E-14	3.1524E-13	1.8638E-13	-2.877E-16	2.951E-13	1.363E-12	5.224E-09	3.898E-13	-2.999E-13
C4H	1.8179E-17	8.0964E-17	4.1596E-17	-7.310E-20	7.623E-17	3.582E-16	1.433E-12	-1.320E-16	-7.287E-17
C2H2	5.5209E-14	1.3052E-13	9.2936E-14	-1.476E-16	1.721E-13	4.646E-13	1.046E-09	2.982E-12	-1.753E-13
HO	9.9985E-06	1.5440E-05	1.3471E-05	-7.470E-09	1.019E-05	-1.954E-05	-2.610E-01	2.742E-04	-1.561E-05
C3	2.3139E-10	7.5703E-10	4.5379E-10	-5.493E-13	4.941E-10	3.586E-09	1.605E-05	-7.929E-09	-5.592E-10

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(c) Incremented Negative Charge Mass Fraction

			DERIVITIVES OF MOLE FR. WITH RESPECT TO --							
				TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$	$\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
NAME	MOLE FR	MASS FR	Z POT.	9.000E 03	1.000E 00	1.753E-01	6.500E-07	2.020E-02	5.908E-01	2.138E-01
C	1.4828E-01	1.6348E-01	1.6799E-01	-1.205E-05	6.466E- 3	7.142E-11	2.797E -3	-1.673E 00	-1.181E- 1	-1.996E-01
E-	2.3771E-02	1.2[illegible]1E-06	1.8224E-04	1.376E-05	-7.083E-03	2.054E-02	1.356E 04	-1.804E-01	-1.107E-02	-1.042E-02
H	2.1840E-01	2.7199E-02	7.1661E-02	-5.164E-06	2.927E- 3	-2.[illegible]67E-01	-3.[illegible]36E -3	8.418E 00	-1.691E-01	-1.495E-01
N	4.4861E-01	5.7684E-01	5.4887E-01	6.067E-07	-2.044E-03	-4.168E-01	-5.323E 03	-4.828E 00	4.039E-01	-3.021E-01
O	1.4387E-01	2.1130E-01	1.8812E-01	-1.672E-06	7.885E- 4	-1.416E-11	-1.835E -3	-1.565E 00	-1.107E-01	5.753E-01
C2	1.7950E-05	3.3598E-05	2.8773E-05	-1.961E-08	1.952E-05	1.730E-04	6.776E-01	-4.053E-04	-2.861E-05	-2.654E-05
H2	8.0876E-06	1.4959E-06	3.7529E-06	-5.959E-09	8.374E- 6	-1.531E-05	-2.249E- 1	6.235E-04	-1.252E-05	-1.108E-05
N2	4.4586E-03	1.1466E-02	7.7145E-03	-6.796E-06	4.418E-03	-8.285E-03	-1.058E 02	-9.597E-02	8.029E-03	-6.004E-03
O2	1.7714E-06	5.2031E-06	3.2756E-06	-1.366E-09	1.791E- 6	-3.488E-06	-4.519E- 2	-3.853E-05	-2.725E- 6	1.417E-05
C+	9.[illegible]984E-03	1.[illegible]031E-02	1.0307E-02	1.093E-05	-5.990E-03	3.596E-02	-5.019E 03	-3.360E-02	-3.009E-03	-2.734E-03
N+	1.4663E-03	1.8853E-03	1.7939E-03	2.594E-06	-1.[illegible]36E-03	-2.629E-03	-8.539E -2	-4.652E-03	2.003E-03	-3.444E-04
O+	3.3144E-04	4.8676E-04	4.3338E-04	5.491E-07	-2.309E-04	-6.126E-04	-1.933E 02	-1.089E-03	-1.005E-04	1.471E-03
CHN	2.7483E-08	6.8180E-08	4.67[illegible]5E-08	-5.714E-11	5.641E-08	8.[illegible]84E-08	-1.897E-4	4.534E-07	-1.842E-08	-5.763E-08
CN	3.3444E-04	7.9876E-04	5.5767E-04	-3.977E-07	3.475E-04	1.300E-03	2.342E 00	-7.373E-03	3.470E-05	-4.724E-04
CO	1.2271E-03	3.1552E-03	2.1231E-03	-2.208E-06	1.287E-03	4.703E-03	7.500E 00	-2.719E-02	-1.921E-03	4.000E-03
NO	1.0980E-04	3.0244E-04	1.9662E-04	-1.131E-07	1.099E-04	-2.101E-04	-2.703E 00	-2.376E-03	1.441E-05	3.652E-04
C2H	2.9672E-09	6.8171E-09	4.8526E-09	-5.928E-12	6.233E-09	2.578E-08	7.[illegible]70E-5	4.741E-08	-7.024E-09	-6.417E-09
C3H	1.0836E-13	3.6843E-13	2.1559E-13	-3.319E-16	3.407E-13	1.463E-12	4.627E-9	5.[illegible]87E-13	-3.428E-13	-3.144E-13
C4H	2.2137E-17	9.9672E-17	5.[illegible]682E-17	-8.881E-20	9.271E-17	4.056E-16	1.363E-12	-1.459E-16	-8.767E-17	-8.059E-17
C2H2	5.9935E-14	1.4324E-13	9.9973E-14	-1.600E-16	1.866E-13	4.639E-13	5.949E-10	3.268E-12	-1.883E-13	-1.707E-13
HO	9.7804E-06	1.5269E-05	1.3185E-[illegible]5	-7.298E-09	9.965E-06	-1.889E-[illegible]5	-2.6[illegible]7E-1	2.7[illegible]6E-04	-1.509E-05	3.241E-05
C3	2.7044E-10	8.9447E-10	5.3[illegible]67E-10	-6.401E-13	5.763E-10	3.9[illegible]8E-09	1.531E-[illegible]5	-9.154E-09	-6.463E-10	-5.996E-10

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(d) Incremented Nitrogen Mass Fraction

			DERIVITIVES OF MOLE FR.WITH RESPECT TO --						
			TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$	$\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
NAME	MOLE FR	MASS FR	Z POT. 9.000E 03	1.000E 00	1.753E-01	5.500E-07	2.02[illegible]E-02	6.[illegible]8E-01	2.138E-01
C	1.4680E-01	1.6288E-01	1.6581E-01	-1.221E-05	6.571E-03	7.[illegible]96E-01	3.253E-03	-1.648E 00	-1.162E-01
E-	2.2337E-02	1.1349E-06	1.7073E-04	1.403E-05	-7.219E-03	2.266E-02	1.3[illegible]2E-04	-1.624E-01	-9.768E-03
H	2.1702E-01	2.0198E-02	7.0992E-02	-5.207E-06	2.95[illegible]E-03	-2.[illegible]43E-01	-2.890E-03	8.379E 00	-1.669E-01
N	4.5314E-01	5.8637E-01	5.5273E-01	4.960E-07	-2.034E-03	-4.184E-01	-5.047E-03	-4.846E 00	3.975E-01
O	1.4295E-01	2.1129E-01	1.8635E-01	-1.747E-06	8.267E-04	-1.399E-01	-1.727E-03	-1.545E 00	-1.093E-01
C2	1.7603E-05	3.9062E-05	2.8118E-05	-1.929E-08	1.918E-05	1.702E-04	7.801E-01	-3.952E-04	-2.787E-05
H2	7.9855E-06	1.4864E-06	3.6943E-06	-5.839E-09	8.203E-06	-1.504E-05	-2.127E-01	6.167E-04	-1.229E-05
N2	4.5490E-03	1.1773E-02	7.8471E-03	-6.937E-06	4.508E-03	-8.400E-03	-1.013E-02	-9.730E-02	7.982E-03
O2	1.7488E-06	5.1695E-06	3.2243E-06	-1.351E-09	1.769E-06	-3.423E-06	-4.226E-02	-3.780E-05	-2.673E-06
C+	9.5860E-03	1.9635E-02	1.0827E-02	1.102E-05	-6.059E-03	3.661E-02	-5.374E-03	-3.789E-02	-3.397E-03
N+	1.5761E-03	2.0394E-03	1.9225E-03	2.710E-06	-1.074E-03	-3.754E-03	-9.361E-02	-5.397E-03	2.072E-03
O+	3.5045E-04	5.1796E-04	4.5685E-04	5.631E-07	-2.352E-04	-6.986E-04	-2.085E-02	-1.240E-03	-1.146E-04
CHN	2.7310E-08	6.8183E-08	4.6271E-08	-5.685E-11	5.619E-08	8.108E-08	-6.278E-05	4.559E-07	-1.867E-06
CN	3.3446E-04	8.0389E-04	5.5601E-04	-3.984E-07	3.479E-04	1.308E-03	3.686E 00	-7.331E-03	2.864E-05
CO	1.2072E-03	3.1236E-03	2.0822E-03	-2.175E-06	1.268E-03	4.654E-03	1.216E-01	-2.660E-02	-1.878E-03
NO	1.1020E-04	3.0547E-04	1.9674E-04	-1.136E-07	1.103E-04	-2.096E-04	-2.559E 00	-2.370E-03	1.245E-05
C2H	2.8901E-09	6.6822E-09	4.7122E-09	-5.785E-12	6.078E-09	2.522E-08	8.958E-05	4.671E-08	-6.799E-09
C3H	1.0450E-13	3.5755E-13	2.0727E-13	-3.207E-16	3.289E-13	1.417E-12	5.554E-09	5.161E-13	-3.286E-13
C4H	2.1135E-17	9.5767E-17	4.8241E-17	-8.496E-20	8.861E-17	3.887E-16	1.592E-12	-1.328E-16	-8.319E-17
C2H2	5.8067E-14	1.3952E-13	9.6465E-14	-1.551E-16	1.808E-13	4.516E-13	1.025E-09	3.177E-12	-1.811E-13
HO	9.6562E-06	1.5171E-05	1.2978E-05	-7.214E-09	9.843E-06	-1.854E-05	-2.453E-01	2.685E-04	-1.481E-05
C3	2.6245E-10	8.7358E-10	5.1343E-10	-6.227E-13	5.601E-10	3.806E-09	1.745E-05	-8.837E-09	-6.233E-10

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(e) Decremented Pressure

NAME	MOLE FR	MASS FR	Z POT.	DERIVITIVES OF MOLE FR. WITH RESPECT TO -- TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$	$\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
C	1.4726E-01	1.6236E-01	1.6677E-01	-1.307E-05	7.828E-03	7.114E-01	3.361E	-3	-1.668E	-01	-1.178E-01	-1.187E-01
E-	2.3219E-02	1.1723E-06	1.7794E-	4 1.484E-05	-8.484E-03	2.441E-02	1.298E	04	-1.685E-01	-1.1	0E-02	-9.584E-03
H	2.1839E-01	2.0198E-02	7.1631E-	2 -5.204E-06	3.246E-03	-2.975E-01	-2.9	3E 03	8.418E	00	-1.694E-01	-1.497E-01
N	4.4929E-01	5.7775E-01	5.4953E-	1 -1.039E-06	-1.225E-	3 -4.192E-01	-4.977E	03	-4.846E	00	4.045E-01	-3.034E-01
O	1.4396E-01	2.1144E-01	1.8817E-01	-1.984E-06	1.049E-03	-1.416E-01	-1.729E	03	-1.567E	00	-1.11 E-	1 5.755E-01
C2	1.5941E-05	3.5152E-	5 2.5531E-	5 -1.764E-08	1.941E-05	1.540E-04	7.319E-01	-3.612E-04	-2.551E-	5	-2.353E-05
H2	7.2781E-06	1.3462E-06	3.3760E-06	-5.365E-09	8.303E-06	-1.383E-05	-1.935E-	1 5.611E	-04	-1.129E-	5 -9.977E-06
N2	4.0249E-03	1.0351E-	2 6.9615E-	3 -6.165E-06	4.45 E-	3 -7.511E-03	-8.917E	01	-8.682E-02	7.247E-03	-5.436E-03
O2	1.5962E-06	4.6888E-06	2.9505E-06	-1.238E-09	1.797E-	6 -3.139E-	6	-3.833E-	2	-3.475E-05	-2.463E-	6 1.276E-05
C+	1.1278E-02	1.1332E-	2 1.1640E-02	1.165E-05	-7.118E-03	3.885E-02	-5.511E	03	-4.186E-02	-3.753E-03	-3.344E-03
N+	1.6704E-03	2.1479E-03	2.0429E-03	2.849E-06	-1.259E-	3 -3.315E-03	-9.525E	02	-5.895E-03	2.231E-	3 -4.386E-04
O+	3.7724E-04	5.5407E-04	4.93 9E-04	6.015E-07	-2.786E-	4 -7.676E-04	-2.155E	02	-1.369E-03	-1.269E-04	1.664E-03
CHN	2.2140E-08	5.4929E-08	3.7612E-08	-4.628E-11	5.065E-	8 6.525E-08	-3.125E-	5	3.638E-07	-1.495E-	8 -4.647E-08
CN	2.9938E-04	7.1506E-	4 4.9931E-04	-3.593E-07	3.477E-04	1.167E-03	3.557E	00	-6.620E-03	3.000E-05	-4.232E-04
CO	1.0975E-03	2.8220E-03	1.8981E-03	-1.985E-06	1.286E-03	4.222E-03	1.202E	01	-2.438E-02	-1.725E-	3 3.577E-03
NO	9.9030E-05	2.7279E-	4 1.7727E-	4 -1.026E-07	1.1 5E-	4 -1.898E-04	-2.286E	00	-2.146E-03	1.277E-05	3.290E-04
C2H	2.3703E-09	5.4461E-09	3.8751E-09	-4.771E-12	5.555E-	9 2. 65E-08	7.733E-	5	3.766E-08	-5.632E-	9 -5.124E-09
C3H	7.7371E-14	2.6308E-13	1.5387E-13	-2.387E-16	2.714E-13	1.048E-12	4.300E-09	3.528E-13	-2.457E-13	-2.244E-13
C4H	1.4127E-17	6.3613E-17	3.2332E-17	-5.710E-20	6.60 E-17	2.596E-16	1.110E-12	-9.563E-17	-5.617E-17	-5.140E-17
C2H2	4.3088E-14	1.0299E-13	7.1846E-14	-1.157E-16	1.495E-13	3.344E-13	8.330E-10	2.345E-12	-1.358E-13	-1.227E-13
HO	8.8072E-06	1.3750E-05	1.1869E-05	-6.592E-09	9.981E-	6 -1.703E-	5	-2.228E-	1 2.436E-	4	-1.363E-	5 2.917E-05
C3	2.1456E-10	7.0979E-10	4.2087E-10	-5.126E-13	5.110E-10	3.109E-09	1.478E-05	-7.292E-09	-5.150E-10	-4.751E-10

TABLE I

TABLES OF STATE DERIVATIVES OBTAINED BY NICHE

(f) Decremented Temperature

			DERIVITIVES OF MOLE FR.WITH RESPECT TO --						
				TEMP	PRES	$\tilde{K}_C$	$\tilde{K}_E$ - $\tilde{K}_H$	$\tilde{K}_N$	$\tilde{K}_O$
NAME	MOLE FR	MASS FR	Z POT. 8.9[illegible]E 03	1.[illegible]E 00	1.753E-01	5.5[illegible]E-07	2.02[illegible]E-02	5.9[illegible]E-01	2.138E-01
C	1.4915E-01	1.6381E-01	1.6845E-01	-1.112E-05	5.827E-03	7.189E-01	3.065E-03	-1.682E 00	-1.184E-01
E-	2.1086E-02	1.1606E-06	1.6117E-04	1.294E-05	-6.53[illegible]E-03	1.981E-02	1.343E-04	-1.58[illegible]E-01	-9.665E-03
H	2.1923E-01	2.[illegible]197E-02	7.1715E-02	-5.380E-06	3.028E-03	-2.074E-01	-3.0[illegible]9E-03	8.440E 00	-1.698E-01
N	4.4897E-01	5.7510E-01	5.4763E-01	2.990E-06	-3.432E-03	-4.158E-01	-5.241E-03	-4.835E 00	4.[illegible]29E-01
O	1.4420E-01	2.1098E-01	1.8798E-01	-1.275E-06	5.721E-04	-1.430E-01	-1.820E-03	-1.572E 00	-1.[illegible]08E-01
C2	1.9958E-05	4.3841E-05	3.1879E-05	-2.192E-08	2.152E-05	1.924E-04	8.[illegible]93E-01	-4.501E-04	-3.[illegible]70E-05
H2	8.7377E-06	1.61[illegible]3E-06	4.[illegible]422E-06	-6.590E-09	8.979E-06	-1.653E-05	-2.398E-01	6.728E-04	-1.354E-05
N2	5.21[illegible]5E-03	1.[illegible]3349E-02	8.9382E-03	-8.[illegible]53E-06	5.131E-[illegible]3	-9.651E-[illegible]3	-1.216E-02	-1.122E-01	9.351E-03
O2	1.9194E-06	5.6166E-06	3.5386E-06	-1.504E-09	1.935E-06	-3.807E-06	-4.845E-02	-4.184E-05	2.949E-06
C+	8.5476E-03	9.3876E-03	9.6540E-03	1.037E-05	-5.567E-03	3.317E-02	-5.267E-03	-3.235E-02	2.87[illegible]E-03
N+	1.3049E-03	1.6715E-03	1.5917E-03	2.336E-06	-9.108E-04	-2.435E-03	-8.461E-02	-4.277E-03	1.769E-[illegible]3
O+	2.9843E-04	4.3662E-04	3.8903E-[illegible]4	4.989E-07	-2.048E-[illegible]4	-5.764E-04	-1.938E-02	-1.[illegible]17E-03	-9.251E-05
CHN	3.3906E-08	8.3796E-08	5.7446E-08	-7.154E-11	6.935E-08	9.995E-[illegible]8	-1.655E-[illegible]4	5.[illegible]78E-07	-2.276E-08
CN	3.7662E-04	8.9607E-04	6.26[illegible]8E-04	-4.527E-07	3.885E-04	1.466E-03	3.331E-[illegible]3	-8.[illegible]03E-03	3.887E-[illegible]5
CO	1.47[illegible]0E-03	3.7652E-[illegible]3	2.5355E-[illegible]3	-2.684E-06	1.533E-[illegible]3	5.627E-03	1.161E-[illegible]1	-3.260E-02	-2.297E-[illegible]3
NO	1.2210E-04	3.3505E-04	2.1798E-04	-1.275E-07	1.217E-04	-2.342E-04	-2.966E-[illegible]0	-2.646E-03	1.575E-[illegible]5
C2H	3.6188E-09	8.2826E-[illegible]9	5.9[illegible]3E-[illegible]9	-7.324E-12	7.57[illegible]E-[illegible]9	3.146E-[illegible]8	9.883E-[illegible]5	5.77[illegible]E-08	-8.55[illegible]E-[illegible]9
C3H	1.4684E-13	4.9735E-13	2.9124E-13	-4.559E-16	4.597E-13	1.984E-12	7.[illegible]23E-[illegible]9	6.853E-13	-4.635E-13
C4H	3.2939E-17	1.4775E-16	7.5134E-17	-1.339E-19	1.374E-16	6.[illegible]39E-16	2.251E-12	-2.177E-16	-1.301E-16
C2H2	7.8351E-14	1.8655E-13	1.3029E-13	-2.126E-16	2.433E-13	6.[illegible]71E-13	1.[illegible]65E-[illegible]9	4.266E-12	-2.458E-13
HO	1.[illegible]573E-05	1.6444E-05	1.4210E-05	-8.[illegible]30E-09	1.076E-05	-2.[illegible]49E-05	-2.785E-01	2.918E-04	-1.631E-[illegible]5
C3	3.41[illegible]6E-1[illegible]	1.1238E-[illegible]9	6.6722E-1[illegible]	-8.158E-13	7.221E-1[illegible]	4.932E-09	2.[illegible]99E-[illegible]5	-1.154E-08	-8.12[illegible]E-10

REFERENCES

1. Bartlett, E. P., Kendall, R. M., and Rindal, R. A.: A Unified Approximation for Mixture Transport Properties for Multicomponent Boundary-Layer Applications. Aerotherm Report No. 66-7, Part IV, March 14, 1967.

2. Kendall, R. M.: A General Approach to the Thermochemical Solution of Mixed Equilibrium-Nonequilibrium, Homogeneous or Heterogeneous Systems. Aerotherm Report No. 66-7, Part V, March 14, 1967.