ANL-6656
General, Miscellaneous,
and Progress Reports
(TID-4500, 20th Ed.)
AEC Research and
Development Report

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois

BASIC MATERIAL RESULTING FROM
ANL ROCKET STUDY

by

C. Cohn, G. Golden, B. Hoglund,
W. Loewenstein, G. Rosenberg,
D. Sparks, and C. Youngdahl

Reactor Engineering Division

May 1963

Operated by The University of Chicago
under
Contract W-31-109-eng-38
with the
U. S. Atomic Energy Commission

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

FOREWORD

Concepts of nuclear rocket reactors that can serve as alternates to the KIWI family of fueled graphite systems are under investigation at Argonne National Laboratory. During the course of the study, a considerable amount of basic material was generated, the general usefulness of which merits publication. This report is a compilation of such material. Included are thermodynamic calculations of vapor pressure and compatibility with hydrogen, verification of multigroup constants used in reactor physics calculations, relations pertaining to a heat transfer parameter study, a heat transfer coefficient correlation for hydrogen, a FORTRAN subroutine to compute thermal properties of hydrogen, considerations pertaining to reactor control, and fuel element stress analyses.

TABLE OF CONTENTS

	<u>Page</u>
I. SUMMARY OF THERMODYNAMIC PROPERTIES OF MATERIALS CONSIDERED FOR NUCLEAR ROCKETS	9
A. Vapor Pressure of Uranium Dioxide	9
B. Vapor Pressure of Uranium Monosulfide	10
C. Vapor Pressure of Uranium Monocarbide	11
D. Vapor Pressure of Zirconium Monocarbide	13
E. Vapor Pressure of Beryllia.	13
F. Vapor Pressure of Tungsten	14
G. Equilibrium Interaction of Urania with Hydrogen.	15
H. Equilibrium Interaction of Uranium Monosulfide with Hydrogen.	16
I. Equilibrium Interaction of Uranium Monocarbide with Hydrogen.	17
J. Equilibrium Interaction of Zirconium Monocarbide with Hydrogen.	18
K. Equilibrium Interaction of Beryllia with Hydrogen.	19
L. Thermodynamics of Tungsten-Water Reaction	20
M. Uranium Monosulfide-Water Reaction at Room Temperature	25
II. VERIFICATION OF MULTIGROUP CONSTANTS.	27
A. Multigroup Constants	27
B. Correlations with Integral Experiments.	29
1. U^{235} -W Critical Systems.	29
2. Small Tungsten-reflected Systems.	30
3. Larger Dilute Systems.	30
C. Calculated Core Material Bucklings	32
D. Relative Correlations with Integral Experiments.	33
III. RELATIONS PERTAINING TO A HEAT TRANSFER PARAMETRIC STUDY.	40

TABLE OF CONTENTS

	<u>Page</u>
IV. HEAT TRANSFER COEFFICIENT CORRELATION.	50
V. FORTRAN-II SUBROUTINE FOR HYDROGEN PROPERTIES .	54
VI. CONSIDERATIONS PERTAINING TO REACTOR KINETICS AND CONTROL	71
A. Influence of "Period Effect" Phenomena on Design of Nuclear Rocket Systems.	71
B. Bandwidth Considerations in Design of Nuclear Rocket Reactor Systems.	74
VII. THERMAL STRESSES IN REACTOR FUEL PLATES: I. The Plane Strain Elasticity Solution.	76
A. Exact Solution	76
B. Approximations to the Plane Strain Elasticity Solution. . .	92
VIII. THERMAL STRESSES IN REACTOR FUEL PLATES: II. Thermo-elastic Stresses in a Thin, Unconstrained Plate with Time- dependent Uniform Internal Heat Generation, Subjected to a Sudden Change in Environ- mental Temperature	105

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
II-1.	Material Buckling as a Function of Core Composition (US in W).	32
II-2.	Material Buckling as a Function of Core Composition (UO ₂ in Mo)	32
III-1.	Core Effectiveness vs NTU	44
III-2.	Core Parameter Study.	48
IV-1.	Temperature Dependent Properties of Normal Hydrogen. .	51
IV-2.	Local Hydrogen Heat Transfer Coefficient	52
IV-3.	Temperature and Diameter Correction Factors.	53
VI-1.	Comparison of ILES and Period Equilibrium Transfer Function Bode Plots - Gain	72
VI-2.	Comparison of ILES and Period Equilibrium Transfer Function Bode Plots - Phase	72
VI-3.	Incremental Linear Equivalent System for the Neutron Kinetics Equations	73
VII-1.	ϵ^{-mf} vs $\frac{ y }{b}$ for Various Values of mR	99
VIII-1.	Thermal Stresses at the Surface of a Free Plate Heated Symmetrically.	113

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
I-1.	Vapor Pressure of Uranium Dioxide	9
I-2.	Vapor Pressure of Uranium Monosulfide	10
I-3.	Vapor Pressure of Uranium Monocarbide	12
I-4.	Vapor Pressure of Zirconium Monocarbide	13
I-5.	Vapor Pressure of Beryllia	14
I-6.	Vapor Pressure of Tungsten	15
I-7.	P_{H_2O}/P_{H_2} for Equilibrium Reaction $UO_2(s) + 2H_2(g) = U(x)$ + $2H_2O(g)$	16
I-8.	P_{H_2S}/P_{H_2} for Equilibrium Reaction $US(x) + H_2(g) = U(l)$ + $H_2S(g)$	17
I-9.	$P_{CH_4}/P_{H_2}^2$ for Equilibrium Reaction $UC(x) + 2H_2 = U(l)$ + $CH_4(g)$	18
I-10.	$P_{CH_4}/P_{H_2}^2$ for Equilibrium Reaction $ZrC(s) + 2H_2 = Zr(l)$ + $CH_4(g)$	19
I-11.	P_{H_2O}/P_{H_2} for Equilibrium Reaction $BeO(s) + H_2(g) = Be(x)$ + $H_2O(g)$	19
I-12.	K_1 for Reaction $W(s) + 3H_2O(g) = WO_3(g) + 3H_2(g)$	20
I-13.	K_2 for Reaction $W(s) + 3H_2O(g) = WO_3(l) + 3H_2(g)$	21
I-14.	K_3 for Reaction $W(s) + 2H_2O(g) = WO_2(g) + 2H_2(g)$	22
I-15.	K_4 for Reaction $W(s) + 2H_2O(g) = WO_2(s, l) + 2H_2(g)$	24
I-16.	K_5 for Reaction $W(s) + H_2O(g) = WO(g) + H_2(g)$	25
II-1.	Sulfur (16-Group)	28
II-2.	Tungsten (16-Group)	28
II-3.	Tungsten (LASL-1st 5 Groups)	28
II-4.	U^{235} -W Critical Systems	29
II-5.	High-density Uranium Core in Tungsten Reflector	30
II-6.	Central-material-replacement Effects	31
II-7.	Predicted Material Bucklings	33
II-8.	Properties of Basic Critical Assemblies	35
II-9.	Godiva Perturbation Calculations	36

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
II-10.	Jezebel Perturbation Calculations	37
II-11.	ZPR-III-Assembly 5 Perturbation Calculations.	38
II-12.	ZPR-V-5:1 Assembly Perturbation Calculations.	38
III-1.	Intermediate Results	49
V-1.	Specific Heat of Dissociating Hydrogen at One Atmosphere .	58
V-2.	Variation of $(5R'T-h^\circ)$ with Temperature.	62
V-3.	Specific Heat of Normal Hydrogen vs Temperature for $1500 \leq T \leq 3000^\circ\text{K}$	64
V-4.	Specific Heat of Normal Hydrogen vs Temperature for $600 \leq T \leq 1500^\circ\text{K}$	65
V-5.	Specific Heat of Ortho Hydrogen vs Temperature for $100 \leq T \leq 600^\circ\text{K}$	65
V-6.	Specific Heat of Para Hydrogen vs Temperature for $170 \leq T \leq 600^\circ\text{K}$	66
V-7.	Specific Heat of Para Hydrogen vs Temperature for $100 \leq T \leq 170^\circ\text{K}$	67
V-8.	Enthalpy and Entropy for Ortho Hydrogen	67
V-9.	Enthalpy and Entropy for Para Hydrogen.	68
V-10.	Enthalpy and Entropy for Normal Hydrogen	68
V-11.	Beattie-Bridgman Calculations	69
V-12.	FORTTRAN-II Subroutine for Hydrogen Properties	70

BASIC MATERIAL RESULTING FROM ANL ROCKET STUDY

by

C. Cohn, G. Golden, B. Hoglund,
W. Loewenstein, G. Rosenberg,
D. Sparks, and C. Youngdahl

I. SUMMARY OF THERMODYNAMIC PROPERTIES OF MATERIALS CONSIDERED FOR NUCLEAR ROCKETS

G. Golden

A. Vapor Pressure of Uranium Dioxide¹

In the temperature range 1600-2800°K, the vapor pressure over urania is determined by equilibrium of the following reaction:

In this temperature range, the vapor pressure over $\text{UO}_2(\text{s})$ was found to fit the expression:

$$\log_{10} P(\text{mm}) = 13.298 - \frac{3.7195 \times 10^4}{T} + \frac{3.5162 \times 10^6}{T^2} + \frac{2.6178 \times 10^9}{T^3} \quad .$$

The pressures shown in Table I-1 were computed by means of the above equation.

Table I-1

VAPOR PRESSURE OF URANIUM DIOXIDE

T, °K	P, mm	T, °K	P, mm
2273	0.00688	2673	1.03
2373	0.0278	2773	2.92
2473	0.101	2873	7.73
2573	0.337		

¹Ackermann, R. J., P. W. Gilles and R. J. Thorn, High-temperature Thermodynamic Properties of Uranium Dioxide, J. Chem. Phys., 25, 1089-1097 (1956).

B. Vapor Pressure of Uranium Monosulfide²

The total vapor pressure over uranium monosulfide is determined by the following equilibrium processes:

The total vapor pressure is

$$\pi = P_{\text{US}} + P_{\text{U}} + P_{\text{S}} = P_{\text{US}} + P_{\text{U}} \left[1 + \left(\frac{M_{\text{S}}}{M_{\text{U}}} \right)^{1/2} \right] = P_{\text{US}} + 1.367 P_{\text{U}} \quad .$$

For the temperature interval 2134-2416°K,

$$\log_{10} P_{\text{US}} (\text{atm}) = 8.3828 - \frac{3.2839 \times 10^4}{T} \quad ;$$

$$\log_{10} P_{\text{U}} (\text{atm}) = 7.3739 - \frac{2.9636 \times 10^4}{T} \quad .$$

The total pressures in Table I-2 were computed from the above equations, extrapolating where necessary.

Table I-2

VAPOR PRESSURE OF URANIUM MONOSULFIDE

T, °K	P_{US} , atm	P_{U} , atm	π , atm	π , mm Hg
2273	8.616×10^{-7}	2.165×10^{-6}	3.822×10^{-6}	0.00290
2373	3.500×10^{-6}	7.674×10^{-6}	1.399×10^{-5}	0.0106
2473	1.270×10^{-5}	2.455×10^{-5}	4.626×10^{-5}	0.0352
2573	4.168×10^{-5}	7.176×10^{-5}	1.398×10^{-4}	0.1062
2673	1.251×10^{-4}	1.936×10^{-4}	3.898×10^{-3}	0.296
2773	3.471×10^{-4}	4.860×10^{-4}	1.012×10^{-3}	0.769
2873	8.964×10^{-4}	1.144×10^{-3}	2.460×10^{-3}	1.87

²Cater, E. D., P. W. Gilles and R. J. Thorn, Uranium Monosulfide. I. Vaporization Thermodynamics, and Phase Behavior, J. Chem. Phys., 35, 608-618 (1961); Cater, E. D., E. G. Rauh and R. J. Thorn, Uranium Monosulfide. II. Mass Spectrometric Study of Its Vaporization, ibid., 619-624.

C. Vapor Pressure of Uranium Monocarbide

No experimental measurements are available for the elevated-temperature vapor pressure of uranium monocarbide, and hence it is necessary to employ thermodynamic techniques to estimate this quantity as a function of temperature. Consider the two equilibrium processes:

It is anticipated that, at the temperatures of interest, the second of the above processes goes strongly to the right,³ i.e.,

The standard free energy change for the above reaction can be obtained by summation of the corresponding free energy changes ΔF for the following equilibrium reactions:

An expression for ΔF_1° as a function of temperature was derived from the following data furnished by Thorn:⁴

	S_{298}° , eu	S_{2050}° , eu	$H_{298}^\circ - H_0^\circ$, cal/mole	$H_{2050}^\circ - H_0^\circ$, cal/mole
UC(cubic)	14.3	41.6	2,200	27,400

$$\Delta H_f^\circ = -21,700 \text{ cal/mole at } 298^\circ\text{K} \quad ,$$

together with the following data:⁵

	S_{2050} , eu	$H_{298} - H_0$, cal/mole	$H_{2050} - H_0$, cal/mole
C	9.92	251	9,075
U	33.05	1,559	22,807

³Ackermann, R. J., Argonne National Laboratory private communication.

⁴Thorn, R. J., Argonne National Laboratory private communication.

⁵Stull, D. R. and G. C. Sinke, Thermodynamic Properties of the Elements, No. 18 of the Advances in Chemistry Series, American Chemical Society (Nov 1956).

This was done as follows:

$$\begin{aligned}\Delta H_0^\circ &= \Delta H_f^\circ(298) - \Delta [H^\circ(298) - H_0^\circ] = -21,700 - [2,200 - 251 - 1,559] \\ &= -22,090 \text{ cal/mole} \quad .\end{aligned}$$

$$\begin{aligned}\Delta H_f^\circ(2050) &= \Delta H_0^\circ + \Delta [H^\circ(2,050) - H_0^\circ] = -22,090 + [27,400 - 22,807 - 9,075] \\ &= -26,572 \text{ cal/mole} \quad .\end{aligned}$$

$$\Delta S_f^\circ(2050) = 41.6 - 9.92 - 33.05 = -1.37 \text{ eu} \quad .$$

As a close approximation,

$$\Delta F_f^\circ(T) = \Delta H_f^\circ(T_0) - T \Delta S_f^\circ(T_0) \quad ,$$

i.e.,

$$\Delta F_1^\circ = -\Delta F_f^\circ = 26,572 - 1.37 T \quad .$$

Values of ΔF_2° and ΔF_3° are tabulated in Ref. 5. These data together with the following relationships:

$$\log_{10} K = -\Delta F_T^\circ / 2.3026 RT \quad ;$$

$$K = P_U P_C = P_U^2 (M_C/M_U)^{1/2} \quad ;$$

$$\pi = P_U + P_C = P_U [1 + (M_C/M_U)^{1/2}] \quad ,$$

were used to compute the results shown in Table I-3.

Table I-3

VAPOR PRESSURE OF URANIUM MONOCARBIDE

T, °K	ΔF_T° , cal/mole	K, atm ²	π , mm Hg
2300	154960	1.881×10^{-15}	0.852×10^{-4}
2400	148554	2.960×10^{-14}	3.378×10^{-4}
2500	142107	3.767×10^{-13}	1.205×10^{-3}
2600	135755	3.871×10^{-12}	3.863×10^{-3}
2700	129382	3.361×10^{-11}	1.138×10^{-2}
2800	123000	2.505×10^{-10}	3.108×10^{-2}
2900	116615	1.625×10^{-9}	7.919×10^{-2}

In using the above data, it must be recognized that several processes pertaining to the vaporization of uranium monocarbide have not yet

been properly evaluated. These include the importance of the gaseous dicarbide and the diffusion of uranium in the condensed phase.⁴

D. Vapor Pressure of Zirconium Monocarbide⁶

The vaporization of zirconium monocarbide is reported to proceed via the following process:

In the temperature range 2200-2900°K, the effusion partial pressures of zirconium and carbon over congruent ZrC are given by

$$\log_{10} P_{\text{C}}(\text{atm}) = 7.2877 - \frac{3.8586 \times 10^4}{T^{\circ}\text{K}} \quad ;$$

$$\log_{10} P_{\text{Zr}}(\text{atm}) = 7.7282 - \frac{3.8586 \times 10^4}{T^{\circ}\text{K}} \quad .$$

The results shown in Table I-4 were computed by means of the above equations.

Table I-4

VAPOR PRESSURE OF ZIRCONIUM MONOCARBIDE

T, °K	P _C , atm	P _{Zr} , atm	π, atm	π, mm Hg
2200	5.605 × 10 ⁻¹¹	1.546 × 10 ⁻¹⁰	2.107 × 10 ⁻¹⁰	1.601 × 10 ⁻⁷
2300	3.245 × 10 ⁻¹⁰	8.947 × 10 ⁻¹⁰	1.219 × 10 ⁻⁹	9.264 × 10 ⁻⁷
2400	1.623 × 10 ⁻⁹	4.474 × 10 ⁻⁹	6.097 × 10 ⁻⁹	4.634 × 10 ⁻⁶
2500	7.133 × 10 ⁻⁹	1.967 × 10 ⁻⁸	2.680 × 10 ⁻⁸	2.037 × 10 ⁻⁵
2600	2.798 × 10 ⁻⁸	7.716 × 10 ⁻⁸	1.051 × 10 ⁻⁷	7.988 × 10 ⁻⁵
2700	9.922 × 10 ⁻⁸	2.736 × 10 ⁻⁷	3.728 × 10 ⁻⁷	2.833 × 10 ⁻⁴
2800	3.214 × 10 ⁻⁷	8.861 × 10 ⁻⁷	1.208 × 10 ⁻⁶	9.181 × 10 ⁻⁴
2900	9.599 × 10 ⁻⁷	2.647 × 10 ⁻⁶	3.607 × 10 ⁻⁶	2.741 × 10 ⁻³

E. Vapor Pressure of Beryllia

The vapor pressure of beryllia was determined by the effusion method, assuming the vaporization process to be:⁷

⁶Storms, E. K., A Critical Review of Refractories. Part I, Selected Properties of Group-4a, -5a, and -6a Carbides, LAMS-2674 (March 15, 1962).

⁷Erway, N. D. and R. L. Seifert, Vapor Pressure of Beryllium Oxide, J. Electrochem. Soc., 98, 83-88 (1951).

In the temperature range 1950-2150°C, the vapor pressure based upon the above assumption was found to be

$$\log_{10} P(\text{mm}) = 18.50 - \frac{34230}{T} - 2 \log_{10} T, T^{\circ}\text{K} \quad .$$

Table I-5 was computed from the above equation.

Table I-5

VAPOR PRESSURE OF BERYLLIA

T, °K	P, mm Hg	T, °K	P, mm Hg
2000	6.07×10^{-6}	2300	7.83×10^{-4}
2100	3.59×10^{-5}	2400	3.00×10^{-3}
2200	1.80×10^{-4}		

If the vaporization process is

then the total vapor pressure is 0.828 of that given by Table I-5.

A more recent mass spectrometric study of the vapor effusing from a cell containing BeO indicated that, in the range 1900-2400°K, the vapor consisted primarily of Be and O atoms, and $(\text{BeO})_3$ and $(\text{BeO})_4$ molecules.⁸ Thus, the data of Table I-5 are an upper limit to the actual vapor pressure over beryllia.

F. Vapor Pressure of Tungsten⁹

The vaporization of tungsten follows the reaction

The vapor pressure of tungsten as a function of temperature is given in Table I-6.

⁸Chupka, W. A., J. Berkowitz and C. F. Giese, Vaporization of Beryllium with Tungsten, J. Chem. Phys., 30, 827-834 (1959).

⁹Jones, H. A., I. Langmuir and G. M. J. Mackay, The Rates of Evaporation and the Vapor Pressures of Tungsten, Molybdenum, Platinum, Nickel, Iron, Copper and Silver, Phys. Rev., 30, 201 (1927).

Table I-6

VAPOR PRESSURE OF TUNGSTEN

T, °K	P, mm Hg	T, °K	P, mm Hg
2200	7.41×10^{-10}	2600	5.43×10^{-7}
2300	4.85×10^{-9}	2700	2.15×10^{-6}
2400	2.64×10^{-8}	2800	7.38×10^{-6}
2500	1.28×10^{-7}	2900	2.25×10^{-5}

G. Equilibrium Interaction of Urania with Hydrogen

The equilibrium interaction of pure urania and hydrogen is assumed to follow the equation

where

$$\text{x} = \text{s for } T < 1406^\circ\text{K} \quad ;$$

$$\text{x} = \text{l for } T > 1406^\circ\text{K} \quad .$$

The above equation is the sum of the following

Values of ΔF_1° from 298.16 to 1500°K are given in Ref 10. Generally, ΔF° is linear in temperature over a wide range of temperature, i.e.,

$$\Delta F^\circ(T) = \Delta H^\circ(T_0) - T\Delta S^\circ(T_0) \quad .$$

Since this was found to hold for ΔF_1° in the interval from 298.16 to 1500°K, these data were linearly extrapolated to 2000°K. The data for ΔF_2° were obtained from Ref. 11. Table I-7 was prepared from these data.

¹⁰Coughlin, J. P., Contributions to the Data on Theoretical Metallurgy: XII. Heat and Free Energies of Formation of Inorganic Oxides, Bulletin 542, U. S. Bureau of Mines, Washington (1954).

¹¹JANAF Interim Thermochemical Tables, Vols. 1 and 2 (Dec 31, 1960).

Table I-7

P_{H_2O}/P_{H_2} FOR EQUILIBRIUM REACTION
 $UO_2(s) + 2H_2(g) = U(x) + 2H_2O(g)$

T, °K	ΔF_1° , cal/mole	ΔF_2° , cal/mole	ΔF_T° , cal/mole	$P_{H_2O}/P_{H_2}^*$
1300	206000	-84044	121956	5.613×10^{-11}
1400	201900	-81326	120574	3.883×10^{-10}
1500	197700	-78594	119106	2.106×10^{-9}
1600	193500	-75854	117646	9.237×10^{-9}
1700	189300	-73098	116202	3.396×10^{-8}
1800	185100	-70340	114760	1.080×10^{-7}
1900	180900	-67572	113328	3.037×10^{-7}
2000	176700	-64802	111898	7.700×10^{-7}

$$*2 \log_{10} \left(\frac{P_{H_2O}}{P_{H_2}} \right) = - \frac{\Delta F_T^\circ}{2.302585RT}$$

H. Equilibrium Interaction of Uranium Monosulfide with Hydrogen

At temperatures above the melting point of uranium (1406°K), the equilibrium interaction between uranium monosulfide and hydrogen is assumed to follow the equation

where

$$x = s \text{ for } T < 2735^\circ K \quad ;$$

$$x = l \text{ for } T > 2735^\circ K \quad .$$

The above equation is the sum of the following:

$$\begin{array}{rcl}
 US(x) & = & U(g) + S(g) & \Delta F_1^\circ \\
 U(g) & = & U(l) & \Delta F_2^\circ \\
 S(g) + H_2(g) & = & H_2S(g) & \Delta F_3^\circ \\
 \hline
 US(x) + H_2(g) & = & U(l) + H_2S(g) & \Delta F_T^\circ = \Delta F_1^\circ + \Delta F_2^\circ + \Delta F_3^\circ
 \end{array}$$

In the range 1800-2800°K, ΔF_1° is given by²

$$\begin{aligned}
 \Delta F_1^\circ &= -7.53833 \times 10^6 - 1.2232 \times 10^3 T + 0.132119 T^2 + 2.90655 \\
 &\quad \times 10^6 \log_{10} T + 0.29650 T \log_{10} T \quad .
 \end{aligned}$$

Values of ΔF_2° are tabulated in Ref. 5 and ΔF_3° in Ref. 11. These data were used to compute the results shown in Table I-8.

Table I-8

P_{H_2S}/P_{H_2} FOR EQUILIBRIUM REACTION
 $US(x) + H_2(g) = U(l) + H_2S(g)$

T, °K	ΔF_1° , cal/mole	ΔF_2° , cal/mole	ΔF_3° , cal/mole	ΔF_T° , cal/mole	$P_{H_2S}/P_{H_2}^*$
2300	120600	-46822	5513	79291	2.917×10^{-8}
2400	114160	-44278	6682	76564	1.074×10^{-7}
2500	108210	-41706	7845	74349	3.162×10^{-7}
2600	102880	-39204	9010	72686	7.757×10^{-7}
2700	98350	-36669	10170	71851	1.526×10^{-6}
2800	94720	-34151	11328	71897	2.442×10^{-6}
2900	(92130)	-31620	12491	(73001)	(3.148×10^{-6})

$$*\log_{10}\left(\frac{P_{H_2S}}{P_{H_2}}\right) = - \frac{\Delta F_T^\circ}{2.302585RT}$$

I. Equilibrium Interaction of Uranium Monocarbide with Hydrogen

At temperatures above 1406°K the equilibrium interaction of uranium monocarbide with hydrogen is assumed to follow the reaction

where

$$x = s \text{ for } T < 2748^\circ K \quad ;$$

$$x = l \text{ for } T > 2748^\circ K \quad .$$

The above equation is the sum of the following:

Here ΔF_1° is the same as that in Sect. I-C. Values of ΔF_2° are tabulated in Ref. 11. These data were used to compute the results shown in Table I-9.

Table I-9

$P_{CH_4}/P_{H_2}^2$ FOR EQUILIBRIUM REACTION
 $UC(x) + 2H_2 = U(l) + CH_4(g)$

T, °K	ΔF_1° , cal/mole	ΔF_2° , cal/mole	ΔF_T° , cal/mole	$P_{CH_4}/P_{H_2}^2$, atm ⁻¹ x 10 ⁶
2300	23421	39173	62594	1.127
2400	23284	41833	65117	1.174
2500	23147	44483	67630	1.223
2600	23010	47141	70151	1.267
2700	22873	49791	72664	1.312
2800	22736	52440	75176	1.355
2900	22599	55093	77692	1.395

J. Equilibrium Interaction of Zirconium Monocarbide with Hydrogen

At temperatures above the melting point of zirconium (2125°K), the equilibrium interaction of zirconium monocarbide with hydrogen is assumed to follow the equation

This equation is the sum of the following:

In the range 2200-2900°K, ΔF_1° is given by⁶

$$\Delta F_1^\circ = 353126 - 68.710T \quad .$$

Values of ΔF_2° and ΔF_3° are tabulated in the literature⁵ as are values of ΔF_4° .¹¹ These data were used to produce Table I-10.

Table I-10

$P_{CH_4}/P_{H_2}^2$ FOR EQUILIBRIUM REACTION
 $ZrC(s) + 2H_2 = Zr(l) + CH_4(g)$

T, °K	ΔF_1° , cal/mole	ΔF_2° , cal/mole	ΔF_3° , cal/mole	ΔF_4° , cal/mole	ΔF_T° , cal/mole	$P_{CH_4}/P_{H_2}^2$, atm ⁻¹ x 10 ⁸
2300	195093	-70439	-84717	39173	79110	3.042
2400	188222	-67444	-80992	41833	81619	3.698
2500	181351	-64465	-77254	44483	84115	4.436
2600	174480	-61466	-73541	47141	86614	5.245
2700	167609	-58491	-69840	49791	89069	6.176
2800	160738	-55510	-66113	52440	91555	7.147
2900	153867	-52524	-62396	55093	94040	8.190

K. Equilibrium Interaction of Beryllia with Hydrogen

The equilibrium interaction of beryllia with hydrogen is assumed to proceed via the following reaction:

where

$$x = s \text{ for } T < 1556^\circ K \quad ;$$

$$x = l \text{ for } T > 1556^\circ K \quad .$$

The above reaction is the sum of the following:

Values of ΔF_1° and ΔF_2° are tabulated in the literature.¹¹ Table I-11 was prepared by means of these data.

Table I-11

P_{H_2O}/P_{H_2} FOR EQUILIBRIUM REACTION
 $BeO(s) + H_2(g) = Be(x) + H_2O(g)$

T, °K	ΔF_1° , cal/mole	ΔF_2° , cal/mole	ΔF_T° , cal/mole	P_{H_2O}/P_{H_2}
1000	119687	-46040	73647	8.040×10^{-17}
1100	117388	-44712	72676	3.642×10^{-15}
1200	115101	-43371	71730	8.646×10^{-14}
1300	112820	-42022	70798	1.254×10^{-12}
1400	110545	-40663	69882	1.234×10^{-11}
1500	108276	-39297	68979	8.918×10^{-11}
1600	105932	-37927	68005	5.145×10^{-10}
1700	103491	-36549	66942	2.480×10^{-9}
1800	101057	-35170	65887	1.002×10^{-8}
1900	98626	-33786	64840	3.484×10^{-8}
2000	96200	-32401	63799	1.068×10^{-7}

L. Thermodynamics of Tungsten-Water Reaction

In this section, the equilibrium interaction of tungsten with water vapor in the range 2000-2800°K is studied. Consider, first, the reaction yielding gaseous WO_3 :

This reaction is the sum of the following:

where

$$\Delta F_1^\circ = \Delta F_2^\circ + \Delta F_3^\circ \quad .$$

The value of ΔF_2° is computed from the expression

$$\Delta F_2^\circ = -75700 + 15.54T$$

as given by Ackermann and Thorn.¹² The value of ΔF_3° is given in Ref. 11. Table I-12 was computed from these data.

Table I-12

K_1 FOR REACTION $\text{W(s)} + 3\text{H}_2\text{O(g)} = \text{WO}_3\text{(g)} + 3\text{H}_2\text{(g)}$

T, °K	ΔF_2° , cal/mole	ΔF_3° , cal/mole	ΔF_1° , cal/mole	K_1 , atm
2000	-44620	97203	52583	1.796×10^{-6}
2100	-43066	93036	49970	6.307×10^{-6}
2200	-41512	88863	47351	1.979×10^{-5}
2300	-39958	84687	44729	5.623×10^{-5}
2400	-38404	80496	42092	1.470×10^{-4}
2500	-36850	76317	39467	3.548×10^{-4}
2600	-35296	72120	36824	8.032×10^{-4}
2700	-33742	67923	34181	1.712×10^{-3}
2800	-32188	63726	31538	3.455×10^{-3}

Next, consider the reaction yielding liquid WO_3 (the melting point of WO_3 is 1745°K):

¹²Ackermann, R. J. and R. J. Thorn, Prog. Ceram. Sci. 1, Ch. 2, (1961).

which is the sum of the following reactions:

In computing ΔF_5° , use was made of the well-established approximation

$$\Delta F^\circ(T) = \Delta H^\circ(T') - T \Delta S^\circ(T') \quad .$$

In the calculation T' was taken to be 2000°K; the values of $\Delta H_5^\circ(2000)$ and $\Delta F_5^\circ(2000)$ are -74200 and -86250 cal/mole, respectively.¹³ From these data $\Delta S_5^\circ(2000)$ was computed to be -43.975 eu, and

$$\Delta F_5^\circ(T) = -174200 + 43.975T \quad .$$

Table I-13 was prepared by means of these data.

Table I-13

K_2 FOR REACTION $W(s) + 3H_2O(g) = WO_3(l) + 3H_2(g)$

T, °K	ΔF_5° , cal/mole	ΔF_3° , cal/mole	ΔF_4° , cal/mole	K_2	P_{WO_3} , atm*
2000	-86250	97203	10953	6.356×10^{-2}	2.8×10^{-5}
2100	-81852	93036	1184	6.857×10^{-2}	9.2×10^{-5}
2200	-77455	88863	11408	7.358×10^{-2}	2.7×10^{-4}
2300	-73057	84687	11630	7.852×10^{-2}	7.2×10^{-4}
2400	-68660	80496	11836	8.361×10^{-2}	1.8×10^{-3}
2500	-64262	76317	12055	8.835×10^{-2}	4.0×10^{-3}
2600	-59865	72120	12255	9.331×10^{-2}	8.6×10^{-3}
2700	-55467	67923	12456	9.813×10^{-2}	1.7×10^{-2}
2800	-51070	63726	12656	1.029×10^{-1}	3.4×10^{-2}

$$*P_{WO_3} = K_1/K_2.$$

Since the vapor pressure of WO_3 is relatively low in the range from 2000 to 2800°K, extensive interaction of tungsten and H_2O to form WO_3 will yield the latter largely as the liquid. For this reaction, the equilibrium ratio of the hydrogen to the water partial pressure is

$$P_{H_2}/P_{H_2O} = \sqrt[3]{K_2} \quad .$$

¹³King, E. G., W. W. Weller and A. U. Christensen, Thermodynamics of Some Oxides of Molybdenum and Tungsten, Bureau of Mines Report of Investigation 5664 (March 1960).

This ratio varies from 0.399 at 2000°K to 0.469 at 2800°K. Hence, at 2000°K, as long as the H₂O concentration is less than or equal to 71.5 v/o, equilibrium interaction between tungsten and H₂O to yield liquid WO₃ cannot occur. The same is true at 2800°K for the H₂O concentration less than or equal to 68.1 v/o.

Consider, next, the W-H₂O reaction to yield gaseous WO₂:

This reaction is the sum of the following:

The value of ΔF_7° is given by Ackermann and Thorn¹² as

$$\Delta F_7^\circ = 7360 - 5.80T \quad (2000-2500^\circ\text{K}) \quad .$$

These data were used to prepare Table I-14.

Table I-14

K₃ FOR REACTION $\text{W(s)} + 2\text{H}_2\text{O(g)} = \text{WO}_2\text{(g)} + 2\text{H}_2\text{(g)}$

T, °K	ΔF_7° , cal/mole	$(2/3) \Delta F_3^\circ$, cal/mole	ΔF_6° , cal/mole	K ₃ , atm ²
2000	-4240	64802	60562	2.412×10^{-7}
2100	-4820	62024	57204	1.113×10^{-6}
2200	-5400	59242	53842	4.483×10^{-6}
2300	-5980	56458	50478	1.599×10^{-5}
2400	-6560	53664	47104	5.138×10^{-5}
2500	-7140	50878	43738	1.502×10^{-4}
2600	-7720	48080	40360	4.051×10^{-4}
2700	-8300	45282	36982	1.016×10^{-3}
2800	-8880	42484	33604	2.384×10^{-3}

The melting point of WO₂, while known to lie above 1900°K, is unknown at present. For the purposes of the following calculations this melting point was taken to be 2400°K. The equation for the W-H₂O interaction to yield either solid or liquid WO₂ is:

This can be written as the sum of the following:

In the region 2000-2400°K the approximation

$$\Delta F_9^\circ(T) = \Delta H_9^\circ(2000) - T\Delta S_9^\circ(2000)$$

was used. At 2000°K, ΔF_9° and ΔH_9° are -57600 and 133400 cal/mole, respectively.¹³ Thus, $\Delta S_9^\circ(2000)$ is equal to -37.900 eu and

$$\Delta F_9^\circ(T) = -133400 + 37.900T \quad .$$

Since the entropy of fusion for a large number of elements is 2-3 eu/gram-atom, the entropy of fusion per gram-atom of WO_2 is taken to be 2.5 eu. Thus, the total entropy of fusion of WO_2 is $3 \times 2.5 = 7.5$ eu (note that the entropy of fusion of WO_3 is 10.06 eu, as reported in Ref. 13. This corresponds to an entropy of fusion per gram-atom of $10.06/4 = 2.52$.) The heat of fusion at 2400°K is

$$\Delta H_f = T_f \Delta S_f = 2400 \times 7.5 = 18,000 \text{ cal/mole} \quad .$$

Extrapolation of data of ΔH_9° vs T for solid WO_2 gives¹³

$$\Delta H_9^\circ(2400) = -129200 \text{ cal/mole} \quad .$$

Adding the heat of fusion to the above gives $\Delta H_9^\circ = -111200$ cal/mole for liquid WO_2 at 2400°K. Since the standard free energy change is zero for the fusion process, the standard entropy change for the liquid at 2400°K is computed to be

$$\Delta S_9^\circ = - \frac{111200 - 42440}{2400} = -28.650 \text{ eu} \quad .$$

Then, the standard free energy change at 2400°K or greater is given by

$$\Delta F_9^\circ(T) = 111200 + 28.650T \quad .$$

These equations were used to compute the results shown in Table I-15.

Table I-15

$$K_4 \text{ FOR REACTION } W(s) + 2H_2O(g) = WO_2(s, \ell) + 2H_2(g)$$

T, °K	ΔF_9° , cal/mole	$(2/3) \Delta F_3^\circ$, cal/mole	ΔF_8° , cal/mole	K_4 , atm	P_{WO_2} , atm*
2000	-57600	64802	7202	0.1633	1.5×10^{-6}
2100	-53810	62024	8214	0.1397	8.0×10^{-6}
2200	-50020	59242	9222	0.1213	3.7×10^{-5}
2300	-46230	56458	10228	0.1067	1.5×10^{-4}
2400	-42440	53664	11224	0.0951	5.4×10^{-4}
2500	-39575	50878	11303	0.1028	1.5×10^{-3}
2600	-36710	48080	11370	0.1107	3.7×10^{-3}
2700	-33845	45282	11437	0.1187	8.6×10^{-3}
2800	-30980	42484	11504	0.1265	1.9×10^{-2}

$$*P_{WO_2} = K_3/K_4.$$

As with the WO_3 , the fact that the vapor pressure of WO_2 is relatively low in the range 2000-2800°K indicates that the latter will form largely as the solid or liquid, rather than as the gas. In this case, the equilibrium ratio of the hydrogen to the water partial pressure is

$$P_{H_2}/P_{H_2O} = \sqrt{K_4}.$$

In the range 2000-2800°K, P_{H_2}/P_{H_2O} has its maximum value, 0.404, at 2000°K and its minimum value, 0.308, at 2400°K. Hence, at 2000°K, as long as the H_2O concentration is less than or equal to 71.2 v/o, interaction of tungsten and H_2O to give WO_2 will not occur. Similarly, at 2400°K, if the H_2O concentration is less than or equal to 76.5 v/o, reaction will not occur.

The W- H_2O reaction yielding gaseous WO is considered next (WO exists only as a gas). To do this, free energy functions ($F^\circ - H_0^\circ$) are found as a function of temperature for gaseous WO, O, and W. These are used to compute $\Delta(F^\circ - H_0^\circ)$ for the reaction

From the known value of ΔH_0° for the above reaction, $\Delta F_{10}^\circ = \Delta(F^\circ - H_0^\circ) + \Delta H_0^\circ$ is computed. Then, the standard free energy changes for the reactions

and

are added to the above value to give the standard free energy change for the reaction

Finally, the standard free energy change for the reaction

is added to give the standard free energy change for

The results of these calculations are summarized in Table I-16. They show that:

$$K_5 = P_{H_2} P_{WO} / P_{H_2O}$$

is only 1.1×10^{-5} at $2500^\circ K$; hence, the W- H_2O interaction to produce gaseous WO is negligible.

Table I-16

K_5 FOR REACTION $W(s) + H_2O(g) = WO(g) + H_2(g)$

T, °K	$(F^\circ - H_2^\circ)_{WO, 14}$ cal/mole	$(F^\circ - H_2^\circ)_{O, 5}$ cal/mole	$(F^\circ - H_2^\circ)_{W, 5}$ cal/mole	$\Delta(F^\circ - H_2^\circ)$ cal/mole	$\Delta F_{10}^\circ, 14$ cal/mole	$\Delta F_{11}^\circ, 5$ cal/mole	$\Delta F_{12}^\circ, 5$ cal/mole	ΔF_{13}° cal/mole	$\Delta F_{14}^\circ, 11$ cal/mole	ΔF_{15}° cal/mole	K_5 , atm
2000	-135080	- 86013	- 97054	47987	-106013	29091	130677	53755	32401	86156	3.853×10^{-10}
2100	-142800	- 90835	-102716	50751	-103249	27477	127048	51276	31012	82288	2.733×10^{-9}
2200	-150568	- 95677	-108426	53535	-100465	25876	123433	48844	29621	78465	1.606×10^{-8}
2300	-158424	-100536	-114158	56270	- 97730	24292	119828	46390	28229	74619	8.126×10^{-8}
2400	-166296	-105433	-114848	53985	-100015	22679	116206	38870	26832	65702	1.041×10^{-6}
2500	-174225	-110343	-115538	51656	-102344	21060	112568	31284	25439	56723	1.100×10^{-5}

M. Uranium Monosulfide-Water Reaction at Room Temperature

The reaction of uranium monosulfide with water vapor in air is assumed to follow the equation

This equation is the sum of the following:

¹⁴De Maria, G., et al., Mass Spectrometric Study of Gaseous Molybdenum, Tungsten and Uranium Oxides, J. Chem. Phys., 32, 1373 (1960).

ΔF_1° is estimated from the approximation

$$\Delta F^\circ(T) = \Delta H^\circ(T_0) - T\Delta S^\circ(T_0) \quad .$$

Here, $T_0 = 2300^\circ\text{K}$, $\Delta H^\circ(T_0) = 271,200 \text{ cal/mole}$; $\Delta S^\circ(T_0) = 65.49 \text{ cal/(mole)}(^\circ\text{K})$ (see Ref. 2). Then, for $T = 298^\circ\text{K}$, $\Delta F_1^\circ(298) = 251,684 \text{ cal/mole}$. ΔF_2° and ΔF_4° are taken from Ref. 5, ΔF_3° from Ref. 10, and ΔF_5° and ΔF_6° are taken from Ref. 11. Summation of the values gives

$$\Delta F_T^\circ = -101,900 \text{ cal/mole} \quad .$$

Then,

$$\log \left(\frac{P_{\text{H}_2\text{S}}}{P_{\text{H}_2\text{O}} P_{\text{O}_2}^{1/2}} \right) = \frac{(101900)}{(2.302585)(1.98726)(298.15)} = 74.6911 \quad .$$

Thus, the above equilibrium reaction proceeds strongly to the right.

II. VERIFICATION OF MULTIGROUP CONSTANTS

W. Loewenstein and C. Cohn

A. Multigroup Constants

The fairly large spectral and material variation in anticipated parametric neutronic studies dictated severe requirements on the choice of a set of initial or interim multigroup constants. No single set of constants was found which provided all materials of interest as well as constants for the whole range of neutron energies from fast (≤ 10 Mev) to thermal. Even if such a set (or sets) of constants were available, the degree of validity and the extent of applicability should be the subject of intensive exploratory analysis. The compilation of such a set of constants with all the degrees of freedom required for subsequent analyses is a major objective for future work. This would involve the basic construction of the constants with their accompanying analysis as well as the performance of critical experiments with systems operating on predominantly fast and intermediate-energy neutrons. The experiments would have to fall in a category that has not been extensively investigated in the past. This would include tungsten-based cores with light-density reflectors. With encouragement from materials research, the experimental program could be extended to include mixed carbide cores with light density reflectors.

The sixteen-group constants of Hansen and Roach¹⁵ were used for most of the analyses. This compilation does not include all materials of interest. Sulfur and tungsten cross sections were compiled.¹⁶ These are tabulated in Tables II-1 and II-2, respectively. Subsequently, LASL produced (see Table II-3) some six-group tungsten cross sections.¹⁷ The group structure of the first five groups is identical with that of the sixteen-group constants. Therefore, the reference tungsten investigations used LASL parameters in the five most energetic groups with ANL constants for the less energetic groups. Some comparisons between theory and experiment utilizing these constants are cited in Section II-B. Section II-C summarizes some bare-core, multigroup, fundamental-mode analyses with the same constants. Additional comparisons between experiment and theory utilizing other constants that have been used for nuclear rocket calculations are given in Section II-D.

¹⁵ Hansen, G. E., and W. H. Roach, Six and Sixteen Group Cross Sections for Fast and Intermediate Critical Assemblies, LAMS-2543 (Nov 1961).

¹⁶ O'Shea, D. M., ANL private communication.

¹⁷ Hansen, G. E. and H. Paxton, LASL private communication.

Table II-1

SULFUR (16-GROUP)

Group E _L ^a	σ_{tot}, b	σ_{nonel}, b	σ_{el}, b	$\sigma_{n\gamma}, b$	σ_{nn}, b	ξ	σ_{tr}, b	$\sigma_{j \rightarrow j+1}, b$
1 3.0 Mev	2.40	1.030	1.37	0.530	0.5	0.0386	1.89	0.106
2 1.4 Mev	2.51	0.070	2.44	0.070		0.0337	1.41	0.102
3 0.9 Mev	2.10	0.027	2.07	0.027		0.0355	1.23	0.140
4 0.4 Mev	2.00	0.037	1.96	0.037		0.0385	2.67	0.093
5 0.1 Mev	3.32	0.080	3.24	0.080		0.0489	0.63	0.115
6 0.017 Mev	0.66	0.025	0.63	0.025		0.0588	1.20	0.021
7 0.003 Mev	1.20	0	1.20	0		0.0612	1.20	0.042
8 550 ev	1.20	0	1.20	0		0.0612	1.20	0.043
9 100 ev	1.20	0.001	1.20	0.001		0.0612	1.20	0.043
10 30 ev	1.20	0.006	1.20	0.006		0.0612	1.20	0.061
11 10 ev	1.20	0.015	1.18	0.015		0.0612	1.20	0.068
12 3 ev	1.20	0.033	1.17	0.033		0.0612	1.20	0.060
13 1 ev	1.20	0.060	1.14	0.060		0.0612	1.20	0.063
14 0.4 ev	1.20	0.110	1.09	0.110		0.0612	1.20	0.072
15 0.1 ev	1.25	0.190	1.06	0.190		0.0612	1.25	0.046
16 Thermal	1.40	0.470	0.93	0.470		0.0612	1.40	

^a Lower energy boundary of group

Table II-2

TUNGSTEN (16-GROUP)

Group E _L ^a	σ_{tot}, b	σ_{nonel}, b	σ_{el}, b	$\sigma_{n\gamma}, b$	ξ	σ_{nn}, b	σ_{tr}, b	$\sigma_{j \rightarrow j+1}^{\text{el}}, b$	$\sigma_{j \rightarrow j+1}^{\text{inel}}, b$	$\sigma_{j \rightarrow j+2}^{\text{inel}}, b$	$\sigma_{j \rightarrow j+3}^{\text{inel}}, b$
1 3.0 Mev	5.98	2.500	3.48	0.0178	0.00264	2.480	3.36	0.018	0.684	0.704	1.022
2 1.4 Mev	7.00	2.570	4.43	0.0320	0.00356	2.540	4.03	0.021	0.478	1.080	0.729
3 0.9 Mev	6.90	2.300	4.60	0.0450	0.00594	2.250	4.83	0.062	0.947	0.911	0.144
4 0.4 Mev	7.00	1.720	5.28	0.0640	0.00713	1.660	5.20	0.046	0.600	0.130	
5 0.1 Mev	8.02	0.590	7.43	0.1150	0.00885	0.475	6.68	0.047			
6 0.017 Mev	10.00	0.233	9.77	0.2330	0.01020		9.51	0.056			
7 0.003 Mev	13.20	0.475	12.72	0.4750	0.01080		13.20	0.079			
8 550 ev	15.10	1.110	14.01	1.1100	0.01080		15.10	0.089			
9 100 ev	21.50	5.130	16.37	5.1300	0.01080		21.50	0.103			
10 30 ev	26.78	14.400	12.38	14.4000	0.01080		26.80	0.112			
11 10 ev	144.00	101.600	42.40	101.6000	0.01080		144.00	0.416			
12 3.0 ev	33.70	22.400	11.30	22.4000	0.01080		33.70	0.102			
13 1.0 ev	8.50	3.500	5.00	3.5000	0.01080		8.50	0.049			
14 0.4 ev	8.80	3.800	5.00	3.8000	0.01080		8.80	0.059			
15 0.1 ev	11.50	6.500	5.00	6.5000	0.01080		11.50	0.039			
16 Thermal	17.50	12.500	5.00	12.5000	0.01080		17.50				

Table II-3

TUNGSTEN (LASL - 1st 5 GROUPS)

Group E _L ^a	σ_{tr}, b	$\sigma_{n\gamma}, b$	$\sigma_{j \rightarrow j}, b$	$\sigma_{j \rightarrow j+1}, b$	$\sigma_{j \rightarrow j+2}, b$	$\sigma_{j \rightarrow j+3}, b$	$\sigma_{j \rightarrow j+4}, b$	$\sigma_{j \rightarrow j+5}, b$
1 3.0 Mev	3.4	0.02	1.20	0.33	0.46	0.79	0.53	0.07
2 1.4 Mev	3.8	0.05	1.76	0.30	0.96	0.64	0.09	
3 0.9 Mev	4.2	0.12	2.73	0.70	0.55	0.10		
4 0.4 Mev	5.2	0.12	4.60	0.40	0.08			
5 0.1 Mev	7.0	0.20	6.72	0.08				

^a Lower energy boundary of group

B. Correlations with Integral Experiments

The same multigroup constants used in the unmoderated-system parametric study were tested by comparison with existing pertinent fast-neutron critical-assembly data. Some constituent materials of interest have not, in the past, been extensively studied in fast critical facilities. This subsection cites comparisons between theory and experiment which may be used to establish uncertainties in the results of the unmoderated-system parametric study.

1. U^{235} -W Critical Systems

Several small cylinders of U^{235} diluted with tungsten have been brought to very high multiplication at LASL. These data were then extrapolated to critical and converted to spherical geometry. The unreflected systems were then calculated by means of the DSN program. Table II-4 shows the result of these calculations. The predicted bare core radius obtained from a multigroup fundamental-mode analysis¹⁸ using the leakage criterion of asymptotic transport theory is also shown. It may be seen

Table II-4

U^{235} -W CRITICAL SYSTEMS

Core Composition (v/o)			Critical Mass (kg U)		Predicted Critical Radius (cm)	
U^{235}	U^{238}	W	Experiment*	Predicted**	DSN**	HOBO [†]
93.3	6.7	0	51.6	52.7	8.76	10.91
68.2	4.9	26.9	71.4	72.4	10.81	12.98
53.5	3.8	42.6	91.7	92.3	12.70	14.88
44.1	3.2	52.7	109.6	112.9	14.49	16.66
37.5	2.7	59.8	129.3	135.0	16.23	18.39
32.7	2.3	65.0	151.7	158.9	17.95	20.09
28.8	2.1	69.1	173.7	186.3	19.72	21.86

* Cylindrical results have been converted to spherical geometry;
H. C. Paxton, LASL, private communication.

** Using the DSN method; an approximate numerical solution of the transport equation.

[†] From a multigroup fundamental-mode analysis using the leakage criterion from asymptotic transport theory. The core material buckling κ may be obtained from the equation $\kappa = \pi/r_{\text{HOBO}}$. The extrapolation distance δ may be obtained from $\delta = r_{\text{HOBO}} - r_{\text{DSN}}$.

¹⁸ Okrent, D., et al., A Survey of the Theoretical and Experimental Aspects of Fast Reactor Physics, Proc. 1955 Geneva Conference, Vol. 5, p. 347.

that, as the system size increases (greater W content), there is a tendency to overpredict the required critical mass. If the incurred error in a criticality calculation is related to the material buckling of the system, it is not unreasonable to expect that the reactivity of an unreflected 1500-liter tungsten-bearing system is underpredicted by a few percent.

2. Small Tungsten-reflected Systems

High-density, highly enriched uranium cores were studied with two thicknesses of tungsten reflector. Table II-5 summarizes these results along with corresponding predicted sizes.

These comparisons show that the high-energy transport cross sections in the multigroup constants are reasonable.

Table II-5

HIGH-DENSITY URANIUM CORE IN TUNGSTEN REFLECTOR

Reflector Thickness (in.)	Critical Mass (kg U)	
	Measured*	Predicted**
1.0	31.2	32.4
2.0	24.1	25.4

* Paxton, H. C., Critical Data for Nuclear Safety Guidance, LAMS-2415 (1960).

** DSN calculations.

3. Larger Dilute Systems

Tungsten and other material replacement experiments have been performed on a wide variety of fast-neutron systems investigated at ANL. Typical are the central-material-replacement experiments with Assemblies 38 and 39 of ZPR-III.¹⁹ Assembly 38 was a spherical system with a high-density uranium ($U^{238}/U^{235} \approx 9$) core in a thick, high-density, depleted uranium reflector. Assembly 39 was a spherical system with a relatively low-density core ($U^{238}/U^{235} \approx 1.5$) containing large amounts of iron and aluminum, also surrounded by a thick, high-density uranium reflector. Table II-6 summarizes a comparison between several measured and predicted material-replacement effects at the center of the core.

¹⁹ Bates, J. C., et al., Two Spherical Fast Critical Experiments, ANL-6582 (1962).

Table II-6

CENTRAL-MATERIAL-REPLACEMENT EFFECTS

ZPR-III Assembly No.	Material	Reactivity Effect (in hours/kg)	
		Measured*	Predicted**
39 ($M_C \approx 427 \text{ kg U}^{235}$)	U^{235}	+108	+112
	S	- 6.8	- 22
	W	- 7.7	- 11.2
	Mo	-	- 11.0
38 ($M_C \approx 424 \text{ kg U}^{235}$)	U^{235}	+164	+146
	W	- 14.4	- 15.3
	S	- 19	- 27.3

*Ref. 19

**DSN reactivity calculations

These results show that the multigroup constants are reasonable and the effective capture cross sections are not inappropriate. In general, there is a tendency for predicted tungsten reactivity losses to exceed those actually observed. This implies that predicted critical masses of tungsten-based systems, utilizing these constants, are larger than those in the experimental critical assembly or actual reactor.

The discrepancy between predicted and measured reactivity losses of sulfur is significant by itself. However, in a system analysis each atom of U^{235} is accompanied by only one atom of sulfur. Hence, the discrepancy between predicted and measured $\bar{\sigma}_a$ for U^{235}S will not exceed 10%. In evaluating the neutronics of pure sulfur, it must be considered that the material-replacement sample, which has not been extensively used in the past, may be impure. Preliminary investigations into this matter have at least raised such a question.

These correlations between theory and experiment are quite limited and by no means complete. Additional pertinent experiments are required to predict the neutronic behavior of these systems confidently. Ultimately, this will require the performance of critical experiments involving large quantities of the structural and/or moderating materials to be used in the actual system. These will, in turn, suggest modifications to both reactor analysis and neutronic constants used therein.

C. Calculated Core Material Bucklings

Bare-core, multigroup, fundamental-mode analyses were performed for the US in tungsten and for UO_2 in molybdenum systems. The resulting material bucklings κ^2 are shown as a function of fuel loading in Figs. II-1 and II-2. The material bucklings for the cores used in the parametric survey are also indicated on the figures.

Fig. II-1. Material Buckling as a Function Core Composition (US in W)

Fig. II-2. Material Buckling as a Function of Core Composition (UO_2 in Mo)

These results demonstrate the obvious expectation that the material buckling is a very rapidly varying quantity as a function of fuel loading. This is particularly true for cores with low fuel loadings in the structural matrix. These curves also show that there is a practical lower limit for fuel loading. The lower limit is, of course, determined by the core size and nuclear uncertainties that may be tolerated in the system.

The material buckling κ^2 is related to the spherical bare core radius R and the significant nuclear parameters through the equation

$$\kappa^2 = (\pi/R)^2 \approx 3\Sigma_{\text{tr}}(\nu\Sigma_f - \Sigma_a) \quad ,$$

where Σ_{tr} , $\nu\Sigma_f$, and Σ_a are effective neutron transport, production (fission x neutron yield), and absorption (including fission) cross sections, respectively. It can be seen that rather small uncertainties in the nuclear parameters can have significant effect on the critical volume of a system with a fixed fuel loading. These predicted curves and their rapid variation with fuel loading re-emphasize the importance of verifying and improving the knowledge of all pertinent nuclear parameters, particularly if interest centers upon the larger of the systems featured in the parametric surveys. To illustrate how current existing experimental data differ from those in the parametric study, the predicted LASL U-W system (II-B) bucklings are given in Table II-7. It may be seen that these values of κ^2 are significantly greater than those of the compositions cited on Figs. II-1 and II-2.

Table II-7

PREDICTED MATERIAL BUCKLINGS

(LASL U-W Systems)

Core Composition (v/o)			Predicted Material Buckling κ^2
U ²³⁵	U ²³⁸	W	
93.3	6.7	0	0.0829
68.2	4.9	26.9	0.0586
53.6	3.8	42.6	0.0445
44.1	3.2	52.7	0.0357
37.5	2.7	59.8	0.0292
32.7	2.3	65.0	0.0243
28.8	2.1	69.1	0.0207

D. Relative Correlations with Integral Experiments

Various multigroup constants of interest for nuclear rocket calculations were checked by comparing predicted with measured central-material-replacement experiments. Experimental data were obtained from Jezebel,²⁰ Godiva,²⁰ ZPR-III Assembly 5,²¹ and the 5:1 fast core of ZPR-V.²² Jezebel and Godiva are small, unreflected, high-density plutonium and highly enriched uranium assemblies, respectively. ZPR-III Assembly 5 has neutronics and core configuration similar to those of the Experimental Breeder Reactor-II. The spectrum of the cited ZPR-V core is similar to that of a reactor with a core volume of at least several hundred liters.

²⁰ Engle, L. B., G. E. Hansen, and H. C. Paxton, Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel, Nuc. Sci. and Eng., 8, 543 (1960).

²¹ Long, J. K., et al., Progress in Nuclear Energy, Series II, Reactors, Pergamon Press (1956), Vol. 2, p. 201.

²² Hummel, H. H., et al., Proceedings of the Second UN International Conference on the Peaceful Uses of Atomic Energy, Geneva, Switzerland, 12, 166 (1958).

The multigroup constants are tested by performing a fundamental mode analysis¹⁸ for each system. This analysis yields the materials buckling which can be related to the critical radius of the unreflected system. The calculations also yield the neutron flux ϕ_j and the adjoint flux ϕ_j^* , where j refers to a range of neutron energies. Thus, the various ϕ_j (where $j = 1 \dots 10$ to 16) may be used to construct the inherent neutron spectrum.

Individual materials are then tested in each system by calculating the effective cross section $\bar{\sigma}_a$. For small perturbation,

$$\bar{\sigma}_a = \frac{\sum_{k=1}^J \phi_k^* \sigma_{rk} \phi_k - \sum_{k=1}^J \sum_{j=1}^{k-1} \phi_k^* \sigma_{j \rightarrow k} \phi_j - \left(\sum_{k=1}^J \beta_k \phi_k^* \right) \left(\sum_{k=1}^J \nu_k \sigma_{fk} \phi_k \right)}{\sum_{k=1}^J \phi_k \phi_k^*},$$

where J is the total number of groups, σ_r is the total cross section for removal of a neutron from a group, $\sigma_{j \rightarrow k}$ is the cross section for transfer of a neutron from group j to group k , σ_f is the fission cross section, and β_k is the fraction of fission neutrons born in group k ; ϕ and ϕ^* are the real and adjoint group fluxes, respectively. Note that $\bar{\sigma}_a$ is negative for a material which adds reactivity, and this formulation is restricted to perturbations at the center of the core. The experimental material-replacement measurements are reactivity effects (ρ) which are related to $\bar{\sigma}_a$ as follows:

$$\rho = A \bar{\sigma}_a,$$

where A is a constant that must be evaluated for each system.

The multigroup constants that were tested in this section were based upon sets of 16-group¹⁵ and 13-group²³ compilations. The 16-group tungsten and sulfur constants are those given in Tables II-1 and II-2.

1. System Calculations

It was expected that it would be possible to predict quite accurately the important spectral properties of the unperturbed systems in which the material replacement experiments were conducted. These results are thus only a basis for the more exacting perturbation analysis. Basic system results are cited in Table II-8.

²³ Cooper, R., LASL private communication.

Table II-8

PROPERTIES OF BASIC CRITICAL ASSEMBLIES

	Godiva	Jezebel	ZPR-III-5	ZPR-V-5:1
Material Buckling κ (cm ⁻¹)				
16-group	0.2881	0.3763		
13-group	0.2897	0.3840		
Critical Radius (cm)				
16-group	8.841*	6.67**		
13-group	8.779*	6.50**		
Reported	8.738	6.30		
$\sigma_f U^{235} / \sigma_f U^{238}$				
16-group	6.48	5.46	11.5	22.0
Reported	5.9	5.13	13.4	24.5
$\sigma_{n,\gamma} U^{238} / \sigma_f U^{235}$				
16-group			0.104	0.118
Reported			0.087	0.096

* Extrapolation distance = 2.065 cm; see Reactor Physics Constants, ANL-5800.

** Extrapolation distance = 1.68 cm; see Reactor Physics Constants, ANL-5800.

2. Perturbation Calculations

The effects of perturbations due to small samples are predicted by evaluating both $\bar{\sigma}_a$ and $\bar{\sigma}_a / \bar{\sigma}_a U^{235}$. Results for Godiva, Jezebel, ZPR-III-Assembly 5 and the ZPR-V-5:1 core are given in Tables II-9, II-10, II-11 and II-12, respectively. Experimental results for each of the four systems are given for comparison.

The cited perturbation calculations and experiments are for the center of the respective cores. Thus, the degree of agreement between theory and experiment is not necessarily an indication of how well the neutronics of a system may be predicted when the material is distributed throughout the core and/or reflector of a given conceptual system. However, these comparisons do give insight as to how well the integrated capture and energy-degradation processes (as well as fission where appropriate) are known. For the purposes of the rocket reactor evaluation, the most interesting materials are U²³⁵, tungsten, hydrogen, boron, and beryllium.

Table II-9

GODIVA PERTURBATION CALCULATIONS*

Material	$\bar{\sigma}_a$			$\bar{\sigma}_a/\bar{\sigma}_a U^{235}$		
	16-group	13-group	Reported	16-group	13-group	Reported
U ²³⁵	-1.852	-1.809	-1.860			
U ²³⁸	-0.288 ^a	-0.329 ^b	-0.303	0.156 ^a	0.182 ^b	0.163
U ²³⁸	-0.293	-0.382 ^c	-0.303	0.158	0.211 ^c	0.163
Pu ²³⁹	-3.522	-3.303	-3.553	1.901	1.826	1.910
Pu ²⁴⁰	-2.26		-2.1	1.22		1.13
Th ²³²	-0.101		0.017	0.0545		-0.0938
H	-0.329 ^d	-0.626 ^f	-0.599	0.178 ^d	0.346 ^f	0.320
H	-0.349 ^e	-0.580 ^g	-0.599	0.188 ^e	0.321 ^g	0.320
B	-0.088	-0.032	-0.088	-0.0475	0.0176	-0.0462
C	-0.054	-0.049	-0.028	0.0291	0.0271	0.0161
Be	-0.134	-0.075	-0.093	0.0724	0.0415	0.0489
O	-0.041		-0.012			
Al	-0.044	-0.021	-0.006	0.0237	0.0116	0.0033
Fe	-0.003	0.079	0.006	0.0016	-0.0437	-0.0013
Ni	0.060	-0.111	0.056	-0.0323	0.0613	-0.0295
W	-0.014 ^h	0.014	0.050	0.0075 ^h	-0.0077	-0.0268
W	0.035 ^k		0.050	-0.0188 ^k		-0.0268
Ta		0.133	0.112			

* Experimental data from Engle, L. B., G. E. Hansen, and H. C. Paxton, Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel, Nuc. Sci. and Eng., 8, 543 (1960).

^a n-2n cross section not included

^f Cooper set H⁴

^b Cooper set U²³⁸-C1

^g Cooper set G + 1H

^c Cooper set 28-C2

^h Table II-2

^d dE/E weighting

^k Table II-3

^e fission spectrum weighting

Table II-10

JEZEBEL PERTURBATION CALCULATIONS*

Material	$\bar{\sigma}_a$			$\bar{\sigma}_a/\bar{\sigma}_a U^{235}$		
	16-group	13-group	Reported	16-group	13-group	Reported
U ²³⁵	-1.88	-2.303	-1.81			
U ²³³	-3.16	-3.148	-3.07	1.68	1.37	1.69
U ²³⁸	-0.234 ^a	-0.219 ^b	-0.258	0.124 ^a	0.095 ^b	0.142
U ²³⁸	-0.246	-0.281 ^c	-0.258	0.131	0.122 ^c	0.142
Pu ²³⁹	-3.666	-3.331	-3.600	1.950	1.446	1.980
Pu ²⁴⁰	-2.67		-2.35	1.42		1.29
Th ²³²	-0.024		0.139	0.013		-0.080
H	-0.015 ^d	-0.331 ^f	-0.141	0.008 ^d	0.144 ^f	0.078
H*	-0.019 ^e	-0.312 ^g	-0.141	0.010 ^e	0.135 ^g	0.078
Be	-0.084	-0.031	-0.036	0.045	0.013	0.019
N	-0.09		0.05	-0.05		0.028
O	-0.004		0.023	0.002		-0.012
Al	0.009	-0.006	0.032	-0.005	0.003	-0.018
S	0.13		0.15	-0.070		-0.087
Fe	0.025	0.008	0.049	-0.013	-0.003	-0.027
Ni	0.096	-0.026	0.109	-0.051	0.011	-0.060
Zr	0.08	-0.190	0.07	-0.04	0.083	-0.044
W	0.109 ^h	0.107	0.151**			
W*	0.139 ^k		0.151**			
C	-0.013	-0.014	0.016	0.007	-0.006	-0.009
Mo	0.069	0.044	0.103	-0.037	-0.019	-0.055

* Experimental data from Engle, L. B., G. E. Hansen, and H. C. Paxton, Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel, Nuc. Sci. and Eng., 8, 543 (1960).

** G. Hansen, LASL, Private Communication.

^a n-2n cross section not included

^f Cooper set H⁴

^b Cooper set U²³⁸-C1

^g Cooper set G + 1H

^c Cooper set 28-C2

^h Table II-2

^d dE/E weighting

^k Table II-3

^e fission spectrum weighting

Table II-11

ZPR-III-ASSEMBLY 5 PERTURBATION CALCULATIONS*

Material	$\bar{\sigma}_a$			$\bar{\sigma}_a/\bar{\sigma}_a U^{235}$		
	16-group	13-group	Reported	16-group	13-group	Reported
U^{235}	-1.846	-1.761				
U^{238}	-0.0577 ^a			0.0313 ^a		0.0100
U^{238}	-0.0626			0.0339		0.0100
S	0.0910			-0.0493		-0.0252
Fe	0.00792	-0.0171		-0.00429	0.00971	-0.00792
Mo	0.0695	0.0104		-0.0376	-0.0059	-0.0289
W	0.0649 ^h	0.1015		-0.0352 ^h	-0.0576	-0.0584
W	0.1237			-0.0670 ^k		-0.0584

* Experimental data extracted from Long, J. K., et al., Progress in Nuclear Energy, Series II, Reactors, Pergamon Press (1956), Vol. 2, p. 201.

^a n-2n cross section not included.

^h Table II-2

^k Table II-3

Table II-12

ZPR-V-5:1 ASSEMBLY PERTURBATION CALCULATIONS*

Material	$\bar{\sigma}_a$			$\bar{\sigma}_a/\bar{\sigma}_a U^{235}$		
	16-group	13-group	Reported	16-group	13-group	Reported
U^{235}	-2.179	-2.322				
B	0.232	0.0097		-0.106	-0.004	-0.130
Fe	0.0309	0.0192		-0.0142	-0.0083	-0.0145
Zr	0.0631	0.0234		-0.0290	-0.0101	-0.0209
S	0.0887			-0.0407		-0.0256
W	0.164 ^h	0.189		-0.0752 ^h	-0.0814	-0.0755
W	0.310 ^k			-0.142 ^k		-0.0755

*Experimental data extracted from Hummel, H. H., et al., Proceedings of the Second UN International Conference on the Peaceful Uses of Atomic Energy, Geneva, Switzerland, 12, 166 (1958).

^h Table II-2

^k Table II-3

It is to be expected that a U^{235} perturbation on a U^{235} -fueled system can be well predicted when the overall system size and spectrum are well predicted. This is indeed the case for Godiva and Jezebel.

Since the metal-based reactor will contain significant amounts of tungsten per unit core volume, the effective capture cross section is of

paramount importance. It appears that the high-energy tungsten constants from Table II-3 are preferable to those from Table II-2 for Godiva and Jezebel spectra. The ZPR-III-Assembly 5 measurement lies between predicted values from Tables II-2 and II-3, with somewhat better agreement with predictions from the 13-group set. The tungsten constants from Table II-2 are in good agreement with the ZPR-V experiment. The rather fluctuating nature of agreement between theory and experiment for tungsten suggests that the nuclear constants require considerable study in conjunction with critical experiments utilizing significant quantities of the material.

Hydrogen is a rocket propellant and its reactivity is of importance to the reactor dynamics. The 13-group cross sections are preferable for predicting central-material-replacement effects for this material in Godiva and Jezebel. It is also interesting to note that the spectral weighting of the 16-group cross sections for hydrogen is a small effect compared with the discrepancy between theory and experiment in these very energetic fast-neutron systems.

Natural boron is a potential control material. The 16-group cross sections are quite good for predicting the central-material-replacement effects in both Godiva and the ZPR-V assembly. There is at least some implication from the ZPR-V result that boron reactivity worth is underpredicted (by ~10%) for the conceptual rocket reactor systems.

Beryllium is a potential reflector and/or control material. The 13-group cross sections for beryllium are in better agreement with experiment than are the 16-group constants. However, a firm conclusion pertaining to these cross sections, as well as to those for hydrogen, cannot be made until material-replacement effects in neutron flux gradients (off core center) are studied.

These limited comparisons indicate that the cross sections for most of the fissionable and fertile materials are in essential agreement with experiment. However, many of the other materials show large deviations. These deviations suggest that considerable refinement of nuclear constants is in order to predict the neutronics of systems containing these materials confidently.

ACKNOWLEDGMENT

Acknowledgment is due to Mr. J. White for over-all computational assistance given in this section.

III. RELATIONS PERTAINING TO A HEAT TRANSFER PARAMETRIC STUDY

B. Hoglund

Nomenclature

a	value of ξ at point of maximum temperature
A	area
$\bar{C}_P$	average bulk specific heat
D_c	core diameter
D_e	equivalent diameter
D_o	outside diameter of rod
f_m	Moody friction factor
F_A	axial power (maximum-to-average)
F_P	local power-peaking factor due to nonuniform moderator or fuel distribution
F_R	radial power (maximum-to-average)
$F_{\Delta T}$	product of hot-channel factors affecting the fluid temperature rise
$F_{\Delta T}^E$	engineering factor that accounts primarily for flow distribution, but can also include construction tolerances, uncertainties, etc., in the fluid temperature rise
F_θ	product of hot-channel factors affecting the film temperature drop
F_θ^E	same as $F_{\Delta T}^E$ on film temperature difference
g_c	conversion factor
G	mass flux
h	average convective heat transfer coefficient
k	thermal conductivity
L_c	core length
N_{Bi}	Biot number
N_{PR}	Prandtl number
N_{RE}	Reynolds number
N_{ST}	Stanton number
NTU	"number of transfer units," $hA_{HT}/W\bar{C}_p$

p	porosity
P	pitch distance between center line of adjacent holes
$\Delta P_{\text{dynamic}}$	dynamic pressure
q	total rate of heat generation
q''	heat flux
q'''	power density
t	plate thickness
T	temperature
W	coolant flow rate
X	"effective" length from surface to point of maximum centerline temperature
α	surface area density
β	moderator volume fraction: moderator volume/total volume
γ	structure volume fraction: structure volume/total volume
ϵ	effectiveness
θ	film temperature drop
μ	average bulk viscosity
ξ	nondimensional length, z/L_c
ρ	density

Subscripts

b	bulk
ϕ	centerline
e	exit
f	fluid
FL	flow
HT	heat transfer
i	inlet
m	fuel meat
max	maximum
R	rods

Optimization of a nuclear rocket engine is strongly dependent upon the requirements of the particular mission. While certain mission requirements are universal, optimization at this time is difficult because many of the mission requirements are as yet unspecified. In view of this, it is desirable to have a parametric evaluation of reactors over a range of unknown variables.

The most desirable nuclear rocket reactor would have the highest reliability with the lightest weight and the lowest cost. Past experience has shown that it is unlikely that one reactor will satisfy all of these requirements and that the optimum reactor is the result of many compromises. A parameter study is also of value in determining where the "trade-offs" will provide the greatest benefits.

The parameter study described below was set up to evaluate a range of reactor core and fuel element geometries that would satisfy certain performance requirements. Specifically, this study evaluates the following reactor parameters;

- (a) length;
- (b) diameter;
- (c) pressure drop;
- (d) power density;
- (e) fuel temperature (surface or centerline);
- (f) fuel-element dimensions

for given values of the following:

- (a) reactor power;
- (b) axial power distribution;
- (c) radial maximum-to-average power;
- (d) propellant temperatures;
- (e) dynamic pressure;
- (f) exit pressure;
- (g) flow distribution;
- (h) limiting fuel temperatures;
- (i) fuel thermal conductivity;
- (j) fuel element porosity; and
- (k) fuel-element surface area density.

The parameter study utilizes the effectiveness-NTU concept described by Kays and London²⁴ for two-fluid heat exchangers and modified by Sutherland²⁵ for application to reactor cores. The concept consists of defining the effectiveness of the heat transfer surface as

$$\epsilon = \frac{T_e - T_i}{T_{\max} - T_i} \quad (1)$$

²⁴ Kays, W. M. and A. L. London, Compact Heat Exchangers, National Press, Palo Alto, California (1955)

²⁵ Sutherland, W. A., Optimizing Core Performance, *Nucleonics*, 19 (1), 80-84 (1961).

The effectiveness is a measure of how closely the maximum propellant temperature approaches the limiting core temperature. By expressing the temperature differences in equation (1) in terms of heat balance and heat transfer relations, as shown below, the effectiveness can be expressed in terms of the power distribution and two dimensionless parameters.

One of the dimensionless parameters is the NTU, which is defined as

$$NTU \equiv hA_{HT}/W\bar{C}_P \quad .$$

The NTU stands for "number of transfer units" and is a measure of the "heat transfer size" of the reactor core. The other parameter, the Biot number, represents the ratio of internal thermal resistance of the fuel to the thermal resistance of the coolant at the surface, and is defined as

$$N_{Bi} = hx/k_m \quad .$$

The effectiveness may be expressed in terms of NTU and N_{Bi} by substituting the following expressions into equation (1). The coolant temperature rise equals

$$T_e - T_i = \frac{q}{W\bar{C}_P} = \frac{NTU}{h} \int_0^1 q''(\xi) d\xi \quad . \quad (2)$$

The maximum centerline temperature may be expressed as

$$T_{max} - T_i = \Delta T_{(a)_{coolant}} + \theta_{(a)} + \Delta T_{(a)_{fuel}} \quad , \quad (3)$$

where

$$\Delta T_{(a)_{coolant}} = \frac{NTU}{h} \int_0^a q''(\xi) d\xi \quad ;$$

$$\theta_{(a)} = \frac{q''(a)}{h} \quad ;$$

and

$$\Delta T_{(a)_{fuel}} = \frac{q''(a)N_{Bi}}{2h} \quad .$$

The general expression for the effectiveness becomes

$$\epsilon = \frac{\int_0^1 q''(\xi) d\xi}{\int_0^a q''(\xi) d\xi + q''(a) \left\{ \frac{[1 + \frac{1}{2} N_{Bi}]}{NTU} \right\}} \quad . \quad (4)$$

The axial position of the maximum core temperature, $\xi = a$, is obtained by differentiating $T_{\max}$ with respect to ξ (equation 3), setting it equal to zero, and solving for ξ :

$$\frac{dT_{\max}}{d\xi} = 0 = q''(\xi) + \frac{[1 + \frac{1}{2} N_{Bi}]}{NTU} \frac{d}{d\xi} q''(\xi) \quad (5)$$

For a uniform axial power distribution, $q''(\xi) = \bar{q}''$, $a = 1$, and the effectiveness equals

$$\epsilon = \frac{1}{1 + \frac{[1 + \frac{1}{2} N_{Bi}]}{NTU}} \quad (6)$$

For a sinusoidal distribution, $q''(\xi) = q''_{\max} \sin(\pi \xi)$,

$$a = \frac{1}{\pi} \arctan \left[- \frac{\pi (1 + \frac{1}{2} N_{Bi})}{NTU} \right] ,$$

and the effectiveness is

$$\epsilon = \frac{2}{[1 - \cos(\pi a)] + \frac{[1 + \frac{1}{2} N_{Bi}]}{NTU} \pi \sin(\pi a)} \quad (7)$$

These expressions are plotted in Fig. III-1.

Fig. III-1. Core Effectiveness vs NTU

If the limiting temperature of the system is the surface temperature, the required NTU is evaluated for a given effectiveness from Fig. III-1 by setting the Biot number equal to zero. If the centerline temperature is limiting, the required NTU is obtained by multiplying the abscissa by $[1 + \frac{1}{2} N_{Bi}]$.

Equation (4) expresses the core effectiveness when the radial power distribution is uniform. The effect of nonuniform radial power distributions and "hot-channel factors" may also be included in the analysis by expressing the effectiveness as

$$\epsilon = \frac{\int_0^1 q''(\xi) d\xi}{\int_0^a F_{\Delta T} q''(\xi) d\xi + F_{\theta} q''(a) \frac{[1 + \frac{1}{2} N_{Bi}]}{NTU}} \quad (8)$$

The hot channel factor $F_{\Delta T}$ may be expressed as the product $F_{\Delta T} = F_R F_{\Delta T}^E$, and the factor F_{θ} is commonly expressed as

$$F_{\theta} = F_R F_A F_P F_{\theta}^E$$

For the purpose of this analysis the local peaking factor F_P may be neglected. The axial power ratio factor F_A may be dropped because the axial power distribution is contained in the effectiveness relation (4). With the assumption that $F_{\Delta T}^E = F_{\theta}^E = F^E$ and for the case where the wall temperature is limiting ($N_{Bi} = 0$), the ratio of the effectiveness for uniform radial power to the effectiveness for nonuniform radial power (including hot-channel factors) may be expressed as

$$\epsilon_{\text{uniform}}/\epsilon_{\text{radial}} = F_R F^E \quad (9)$$

For any given F_R and F^E , the above equation and Fig. III-1 may be used to determine (a) the reduction in effectiveness for any given NTU; or (b) the required NTU's for a given core design, a procedure that often proves valuable when physics calculations lag the heat transfer calculations.

When the limiting wall temperature and terminal propellant temperatures have been specified, the effectiveness is calculated from equation (1) and the required NTU obtained from Fig. III-1 or a similar plot if different axial power distributions are being used. The core geometry is then calculated with the aid of the following relations. The mass flux is calculated from

$$G = \sqrt{2gc\rho_e\Delta P_{\text{dynamic}}} \quad (10)$$

The propellant flow rate equals

$$W = q/\bar{C}_P\Delta T \quad (11)$$

The flow area equals

$$A_{FL} = W/G \quad . \quad (12)$$

For a given porosity, the core diameter is calculated from

$$D_c = \sqrt{\frac{4 A_{FL}}{\pi p(1 - \gamma - \beta)}} \quad (13)$$

The fuel-element equivalent diameter equals

$$D_e = 4p/\alpha \quad . \quad (14)$$

The Stanton number is evaluated from

$$N_{ST} = 0.021 \left(N_{RE} \right)_b^{-0.2} \left(N_{PR} \right)^{-2/3} \left(T_w/T_b \right)^{-0.575} \quad , \quad (15)$$

where T_w is the average wall temperature:

$$T_w = \bar{T}_b + \bar{\theta} \quad ,$$

and $\bar{\theta}$ may be evaluated with the NTU, since it can be shown that $NTU = \Delta T_f/\bar{\theta}$.

The Biot number is calculated from

$$N_{Bi} = hx/2k_m \quad , \quad (16)$$

where $h = N_{ST} G \bar{C}_P$.

For plates,

$$x = t = \frac{D_e}{2} \left(\frac{1-p}{p} \right) \quad .$$

For rod bundles in a triangular matrix,

$$x = D_0 = D_e \left(\frac{1-p}{p} \right)$$

For holes in a matrix (triangular lattice),

$$x = D_e \left\{ \left[\frac{2.205 \left(\frac{P}{D_e} \right)^2}{\left[1.1026 \left(\frac{P}{D_e} \right)^2 - 1 \right]} \ln 1.05 \left(\frac{P}{D_e} \right) - 1 \right] \right\} \quad .$$

Further,

$$\left(\frac{P}{D_e}\right)^2 = \frac{\pi}{4 p \sin 60^\circ} \quad .$$

(Note: This expression for x is obtained by reducing the hexagonal cell to a cylindrical cell of the same volume.) Obtain the effectiveness ϵ^+ from Fig. III-1 for

$$NTU^+ = \frac{NTU}{1 + \frac{1}{2} N_{Bi}} \quad (17)$$

and calculate the centerline temperature from

$$T_c = T_i + \frac{(T_e - T_i)}{\epsilon^+} \quad . \quad (18)$$

If the calculated centerline temperature exceeds the limiting centerline temperature, the limiting temperature in the core becomes the centerline temperature, and the calculation must be repeated with the effectiveness as a function of the centerline temperature instead of the wall temperature. The "modified" NTU (NTU^+) is obtained from Fig. III-1 and the true NTU is calculated from equation (17). An iterative calculation is required between equations (15) and (16) until satisfactory convergence is obtained in the NTU.

The core length equals

$$L_c = \frac{(NTU) D_e}{4 (N_{ST})} \quad (19)$$

The pressure drop through the core is calculated from

$$\Delta P = \frac{G^2}{g_c \bar{\rho}} \left[\ln \left(\frac{\rho_i}{\rho_e} \right) + \frac{f_m L_c}{2 D_e} \right] \quad (20)$$

(an iterative calculation between ρ and ρ_i). The power density equals

$$q''' = \frac{4q}{\pi D_c^2 L_c} \quad . \quad (21)$$

Sample Calculation:

The results of a sample calculation utilizing this method are shown below for a plate-type core. The intent was to calculate a variety of core L/D ratios that satisfy all of the imposed limitations. When the mission requirements are specified, one may then pick the core L/D that best fits these requirements. The imposed limitations were the following:

1. Minimum Plate Thickness	0.1016 cm (0.040 in.)
2. Reactor Power	2000 Mw
3. Coolant Temperature	
in	200°K (360°R)
out	2500°K (4500°R)
4. Maximum Dynamic Pressure	
(Mach Number = 0.3 at P = 30 atm	
and T = 2500°K)	1.84 atm (27 psi)
5. Maximum Surface Temperature	2700°K (4860°R)
6. Chamber Pressure	30 atm (441 psia)

The results of the calculation are shown in Fig. III-2. Intermediate results obtained during the calculation are tabulated in Table III-1.

Fig. III-2. Core Parameter Study

Table III-1

INTERMEDIATE RESULTS

ρ	$G,$ gm/(sec)(cm ²)	$D_e,$ cm	NRE	NST	NTU	$L_c,$ cm	$D_c,$ cm	$\Delta P,$ atm
0.2	33.0	0.064	0.86×10^4	3.28×10^{-3}	5.15	24.9	102.4	14.3
0.4	33.0	0.196	2.3×10^4	2.69×10^{-3}	5.15	80.9	72.5	14.0
0.5	33.0	0.254	3.4×10^4	2.48×10^{-3}	5.15	131.8	64.7	13.7
0.6	33.0	0.381	5.1×10^4	2.29×10^{-3}	5.15	214.2	59.1	13.6

The volume fraction of fuel required for criticality was included in Fig. III-2 by utilizing the spherical core criticality calculations and the fast reactor shape factors presented by Loewenstein.²⁶ If, for example, metallurgical studies should reveal that the maximum fuel volume fraction must be less than 40 v/o, Fig. III-2 shows that any of the core L/D ratios between porosities of 0.25 to 0.48 meet the imposed requirements. Which particular L/D is picked would be fixed by other considerations.

²⁶Loewenstein, W. B., and G. W. Main, Fast Reactor Shape Factors and Shape-dependent Variables, ANL-6403 (Nov 1961).

IV. HEAT TRANSFER COEFFICIENT CORRELATION

B. Hoglund

The local heat transfer coefficient to be used in heat transfer calculations with hydrogen can be obtained from the following correlation:

$$\frac{hD}{k_f} = 0.021 \left(\frac{\rho_f D_e V}{\mu_f} \right)^{0.8} \left(\frac{C_p \mu}{k} \right)_f^{0.4} \quad (1)$$

The correlation is the only local heat transfer correlation listed in the summary presented by Hendricks et al.²⁷ It is based on unpublished heat transfer data for hydrogen. Taylor and Kerchegessner²⁸ obtained the same correlation with helium.

Calculation of the heat transfer coefficient from a correlation in which the coolant properties are to be evaluated at the average film temperature is necessarily an iterative process, since the film temperature is a function of the heat transfer coefficient. It is useful, therefore, to have a graphical solution of equation (1) so that the iterative process can be performed rapidly. A graphical solution is obtained by rearranging the correlation as follows.

The modified Reynolds number used in the correlation may be expressed as

$$\frac{\rho_f D_e V}{\mu_f} = \left(\frac{D_e G}{\mu_f} \right) \left(\frac{T_b}{T_f} \right) \quad (2)$$

where $G = \rho_b V$ and $\rho_f / \rho_b = T_b / T_f$ for a perfect gas at a given pressure. Substitution of equation (2) into equation (1) and rearrangement gives

$$h = (0.021)(1.16 \times 10^{-3}) \frac{\text{watt-hr}}{\text{cal}} (3.6 \times 10^3) \frac{\text{sec}}{\text{hr}} \frac{G^{0.8}}{D_e^{0.2}} \left[\left(\frac{C_p}{\mu} \right)_f^{0.4} \left(\frac{T_b}{T_f} \right)^{0.8 k^{0.6}} \right] \quad (3)$$

²⁷Hendricks, R., et al., Correlation of Hydrogen Heat Transfer in Boiling and Supercritical Pressure States, ARS Journal, 244-52 (Feb 1962).

²⁸Taylor, M., and T. Kerchegessner, Measurements of Heat Transfer and Friction Coefficients for Helium Flowing in a Tube at Surface Temperatures up to 5900°R, ARS Journal, 830-92 (1960).

If the bulk temperature T_b is assigned a value of 317°K, the term in the square bracket may be written as

$$\left[\right] = \phi(T_f) T^*$$

where

$$\phi(T_f) = \left[\left(\frac{C_p}{\mu} \right)_f^{0.4} \frac{k^{0.6}}{T_f^{0.8}} \right] \times 10^2 \quad (4)$$

and

$$T^* = (T_b/317)^{0.8} \quad (5)$$

If a value of 0.1 cm is assigned to D_e and a nondimensional diameter-correction factor is defined as

$$D^* = (D_e/0.1)^{-0.2} \quad (6)$$

equation (3) may be written as

$$h = \frac{(0.0877)}{(0.1)^{0.2}} G^{0.8} \phi(T) T^* D^* \quad \text{watts}/(\text{cm}^2)(^\circ\text{K}) \quad (7)$$

Figure IV-1 is a plot of $\phi(T)$ (temperature-dependent properties) vs T_f (average film temperature). The hydrogen properties were obtained from

Fig. IV-1. Temperature-dependent Properties of Normal Hydrogen

King.²⁹ It is recognized that this reference may not be the best available source of hydrogen properties; therefore, Fig. IV-1 may be subject to revision at a later date.

Figure IV-2 is a plot of $\xi = h/T^*D^* = (0.139)G^{0.8} \phi(T_f)$ with $\phi(T)$ as a parameter. The quantity ξ is the local heat transfer coefficient for the special case where $D_e = 0.1$ cm and $T_b = 317^\circ\text{K}$.

Fig. IV-2. Local Hydrogen Heat Transfer Coefficient

The local heat transfer coefficient for any equivalent diameter and bulk temperature is obtained by multiplying ξ by the nondimensional correction factors T^* and D^* . Both T^* and D^* are obtained from Fig. IV-3.

²⁹King, C., Compilation of Thermodynamic Properties, Transport Properties, and Theoretical Rocket Performance of Gaseous Hydrogen, NASA TN-D-275 (April 1960).

Fig. IV-3. Temperature- and Diameter - Correction Factors

In summary, to obtain the local heat transfer coefficient from the correlation expressed by equation (1):

- 1) From Fig. IV-1 obtain $\phi(T)$ for the assumed T_f .
- 2) From Fig. IV-2 obtain ξ as a function of $\phi(T)$ and the mass velocity G .
- 3) Multiply ξ by the values of T^* and D^* obtained from Fig. IV-3.
- 4) Calculate wall temperature and average film temperature.
- 5) Iterate if necessary.

V. FORTRAN-II SUBROUTINE FOR HYDROGEN PROPERTIES

G. Golden and C. Cohn

Nomenclature

R	0.082060 (liter)(atm)/(mole)(°K)
R'	1.98726 cal(thermochemical)/(mole)(°K)
T	temperature, °K
P	total system pressure, atm
P_{H_2}	partial pressure of normal hydrogen, atm
P_H	partial pressure of monatomic hydrogen, atm
ρ	density of real normal hydrogen, moles/liter
ϕ	fractional para content of gas
X	degree of dissociation of normal hydrogen
K	P_H^2/P_{H_2} , equilibrium constant for dissociation, atm
C_O^0	specific heat of ideal ortho hydrogen, cal/(mole)(°K)
C_P^0	specific heat of ideal para hydrogen, cal/(mole)(°K)
C_n^0	specific heat of ideal normal hydrogen, cal/(mole)(°K)
h^0	enthalpy of ideal hydrogen, cal/mole
h	enthalpy of real hydrogen, cal/mole
S^0	entropy of ideal hydrogen at one atmosphere, cal/(mole)(°K)
S	entropy of real hydrogen, cal/(mole)(°K)
S_O^0	entropy of ideal ortho hydrogen at one atmosphere, cal/(mole)(°K)
S_P^0	entropy of ideal para hydrogen at one atmosphere, cal/(mole)(°K)
S_n^0	entropy of ideal normal hydrogen at one atmosphere, cal/(mole)(°K)
ΔF^0	standard free energy change for dissociation, cal/mole
ΔH_d^0	ideal heat of dissociation of hydrogen, cal/mole
ΔE_O^0	difference between internal energy of 2H and H_2 in the rotational-vibrational state $j = 0, v = 0$.

A FORTRAN subroutine has been written to compute the density, enthalpy, entropy, and degree of dissociation of hydrogen in the temperature range 100-3000°K and the pressure range 1-50 atm, given pressure, temperature, and initial ortho-para composition. The assumptions made in establishing this subroutine are as follows:

1. The hydrogen starts at a given para-composition ϕ ; as long as the temperature remains below 600°K , ϕ remains constant at its initial value. At 600°K and above, ϕ is set equal to 0.250.
2. Dissociation of the hydrogen is negligible below 1500°K at pressures of one atmosphere or greater.
3. The Beattie-Bridgman equation is of sufficient accuracy to describe the PVT properties of normal hydrogen in the pressure range of interest and at temperatures in the interval $100^{\circ}\text{K} \leq T \leq 1500^{\circ}\text{K}$.
4. The Beattie-Bridgman constants given in the literature for normal hydrogen³⁰ are equal to those for ortho and para hydrogen, i.e., the difference between the PVT properties of ortho and para hydrogen is negligible.
5. At temperatures of 1500°K and greater, normal hydrogen obeys the perfect gas law.

The first assumption above is closely related to the fact that this subroutine is to be used in calculations of nuclear rocket reactor performance. The feed to such an engine is hydrogen that is stored as the liquid, usually having a high para composition. Equilibrium conversion from the para to the ortho form depends only upon temperature, but such conversion in the absence of special catalysts takes considerable time. Hence, if the hydrogen is heated from, say, 100 to 2500°K in less than 0.01 sec in passing through a reactor core, equilibrium conversion will not take place. Instead, the hydrogen will change directly from its initial to the normal composition at some temperature above 300°K . At temperatures up to 600°K , the enthalpy of ideal ortho hydrogen is greater than that of the ideal para modification due to the heat of the para-ortho conversion, but the average ideal specific heat of the para is greater than that of the ortho variety in this temperature range, so that the two effects tend to cancel each other with increasing temperature. At 600°K , the difference between the enthalpy of the ideal ortho and that of the para form is about 0.001% , and becomes negligible at higher temperatures. Hence, 600°K was taken as the temperature at which instantaneous conversion from the initial to the normal composition occurs.

It is noteworthy that both the enthalpy and entropy of ideal hydrogen at temperatures above 600°K are independent of the temperature at which instantaneous para-ortho conversion is assumed to take place, as long as this temperature is equal to or greater than 600°K . This is because at these higher temperatures the ideal specific heats of the two modifications become equal. As an example of this point, the entropy of normal ideal hydrogen at 1500°K was computed subject to the following assumptions.

³⁰Taylor, H. S., and S. Glasstone, A Treatise on Physical Chemistry. Vol. 2, States of Matter, D. Van Nostrand Co., Inc., (1951).

1. Hydrogen of 80% para content is heated to 600°K, converted to the normal composition at that temperature, and then heated to 1500°K (ideal entropies are tabulated in the literature³¹):

$$\begin{aligned}
 S_n^0(1500^\circ\text{K}) &= \phi S_p^0(600^\circ\text{K}) + (1-\phi) S_o^0(600^\circ\text{K}) + R' \left(\phi \ln \frac{1}{\phi} + [1-\phi] \ln \frac{1}{1-\phi} \right) \\
 &\quad + \int_{600}^{1500} \frac{C_n^0 dT'}{T'} \\
 &= (0.80)(36.083) + (0.20)(38.266) + 0.994 + 45.475 - 38.838 \\
 &= 44.150 \text{ cal}/(\text{mole})(^\circ\text{K}) \quad .
 \end{aligned}$$

2. Hydrogen of 80% para content is heated to 1000°K, converted to the normal composition at that temperature, and then heated to 1500°K:

$$\begin{aligned}
 S_n^0(1500^\circ\text{K}) &= \phi S_p^0(1000^\circ\text{K}) + (1-\phi) S_o^0(1000^\circ\text{K}) + R' \left(\phi \ln \frac{1}{\phi} + [1-\phi] \ln \frac{1}{1-\phi} \right) \\
 &\quad + \int_{1000}^{1500} \frac{C_n^0 dT'}{T'} \\
 &= (0.80)(39.701) + (0.20)(41.884) + 0.994 + 45.475 - 42.455 \\
 &= 44.152 \text{ cal}/(\text{mole})(^\circ\text{K}) \quad .
 \end{aligned}$$

3. Hydrogen of 80% para content is heated to 1500°K and converted to the normal modification:

$$\begin{aligned}
 S_n^0(1500^\circ\text{K}) &= \phi S_p^0(1500^\circ\text{K}) + (1-\phi) S_o^0(1500^\circ\text{K}) + R' \left(\phi \ln \frac{1}{\phi} + [1-\phi] \ln \frac{1}{1-\phi} \right) \\
 &= (0.80)(42.720) + (0.20)(44.903) + 0.994 \\
 &= 44.151 \text{ cal}/(\text{mole})(^\circ\text{K}) \quad .
 \end{aligned}$$

The dissociation of hydrogen is given by the reaction

for which the equilibrium constant,

$$K = \frac{P_H^2}{P_{H_2}} = \frac{4X^2P}{1-X^2} \quad ,$$

³¹Woolley, H. W., R. B. Scott, and F. G. Brickwedde, Compilation of Thermal Properties of Hydrogen in Its Various Isotopic and Ortho-Para Modifications, NBS-RP 1932 (Nov 1948).

depends only upon temperature. Note that the degree of dissociation of the molecular hydrogen, X , is both temperature- and pressure-dependent:

$$X = \sqrt{\frac{K}{4P+K}} \quad .$$

The last equation shows that the degree of dissociation increases with decreasing pressure. Thus, for the range of pressure to be handled by the proposed FORTRAN subroutine, the maximum dissociation encountered will be at one atmosphere for a given temperature.

Rearrangement of the free-energy equation

$$-\Delta F^0 = R'T \ln K = R'T \ln \frac{4X^2P}{1-X^2}$$

leads to

$$\frac{\Delta F^0}{2R'T} + \frac{1}{2} \ln 4P = \ln \left(\frac{1}{X} \right) + \frac{1}{2} \ln (1-X^2) \quad .$$

Hence, for $X^2 \ll 1$, it is seen that $\ln (1/X)$ is linear in $1/T$ at a given pressure. Theoretical values for X at one atmosphere and at temperatures of 1500, 2000 and 3000°K have been computed;³¹ these are 8.675×10^{-6} , 8.125×10^{-4} and 7.850×10^{-2} , respectively. By means of these values it is found that, at one atmosphere,

$$\begin{aligned} X &= 667.42 e^{-27,237.7/T} \quad , \quad 1500^\circ\text{K} \leq T \leq 2000^\circ\text{K} \quad ; \\ &= 732.79 e^{-27,424.5/T} \quad , \quad 2000^\circ\text{K} \leq T \leq 3000^\circ\text{K} \quad . \end{aligned}$$

It might appear that, because of the smallness of the degree of dissociation at one atmosphere and, say, at 2000°K, its effect can be neglected at this temperature. But because the heat of dissociation is so large (108,430 cal/mole H_2), this is not true. Consider the ideal specific heat of the dissociating system:

$$C_d^0 = (1-X) C_n^0 + (2X) \left(\frac{5}{2} R' \right) + \Delta H_d^0 \frac{dX}{dT} \quad .$$

At 2000°K:

$$X = 8.125 \times 10^{-4} \quad ; \quad C_n^0 = 8.195 \quad ;$$

$$\Delta H_d^0 = 103,240 + 5R'T - (H^0 - E_O^0) = 108,430 \text{ cal/mole} \quad ;$$

$$\frac{dX}{dT} = \frac{1.817899 \times 10^7}{T^2} e^{-2.72377/T} = 5.5325 \times 10^{-6}/^\circ\text{K} \quad .$$

Then,

$$C_d^0 = 8.796 \text{ cal}/(\text{mole})(^\circ\text{K})$$

and

$$\frac{C_d^0 - C_n^0}{C_d^0} \times 100\% = 6.8\%$$

The results shown in Table V-1 were computed by means of the above technique. Since dissociation contributes only 0.15% to the specific heat at 1500°K, this effect is neglected at temperatures of 1500°K and below.

Table V-1
SPECIFIC HEAT OF DISSOCIATING HYDROGEN
AT ONE ATMOSPHERE

T, °K	X	C_d^0 , cal/(mole)(°K)	$(C_d^0 - C_n^0)/C_d^0$ %
1500	8.675×10^{-6}	7.731	0.15
1600	2.699×10^{-5}	7.846	0.39
1700	7.346×10^{-5}	7.985	0.94
1800	1.789×10^{-4}	8.167	2.0
1900	3.967×10^{-4}	8.425	3.9
2000	8.125×10^{-4}	8.796	6.8

The virial form of the Beattie-Bridgman equation is³⁰

$$P = \alpha \rho + \beta \rho^2 + \gamma \rho^3 + \delta \rho^4 \quad ,$$

where

$$\alpha = RT \quad ;$$

$$\beta = RTB_0 - A_0 - \frac{Rc}{T^2} \quad ;$$

$$\gamma = -RTB_0b + A_0a - \frac{RB_0c}{T^2} \quad ;$$

$$\delta = RB_0bc/T^2 \quad ,$$

and the Beattie-Bridgman constants for normal hydrogen are

$$A_0 = 0.1975 \quad ;$$

$$a = -0.00506 \quad ;$$

$$B_0 = 0.02096 \quad ;$$

$$b = -0.04359 \quad ;$$

$$c = 504.0 \quad .$$

An equation of state for a gas is generally most in error at low temperatures and high pressures. Hence, it is necessary to examine the accuracy of the Beattie-Bridgman equation at the extreme conditions of temperature and pressure under which the proposed subroutine is to be employed. PVT data for hydrogen have been measured by White and Johnston,³² who fitted their data to the following virial equation:

$$P = A\alpha\rho + B\alpha\rho^2 + C\alpha\rho^3 + D\alpha\rho^4 + E\alpha\rho^5 + F\alpha\rho^6 \quad .$$

In the above equation $A = 1$, and B , C , D , E , and F were evaluated from experimental data in the range from 20.59 to 299.99°K, and by extrapolation to 500°K. The Beattie-Bridgman and White-Johnston equations are compared as follows:

1. Let $T = 100^\circ\text{K}$ and $\rho = 6.000162$ moles/liter. Then, according to the White-Johnston equation,

$$P = 49.5450 \text{ atm and } P/\rho RT = 1.00629.$$

According to the Beattie-Bridgman equation:

$$P = 49.5502 \text{ atm and } P/\rho RT = 1.00635.$$

2. Let $T = 300^\circ\text{K}$ and $\rho = 2.000054$ moles/liter. Then, according to the White-Johnston equation,

$$P = 50.7636 \text{ atm and } P/\rho RT = 1.03100.$$

According to the Beattie-Bridgman equation,

$$P = 50.6814 \text{ atm and } P/\rho RT = 1.02933.$$

(For the same temperature and density, Wooley et al.³¹ give

$$P = 50.7333 \text{ atm and } P/\rho RT = 1.03038.)$$

3. Let $T = 500^\circ\text{K}$ and $\rho = 1.2000324$ moles/liter. Then, according to the extrapolated White-Johnston equation,

$$P = 50.1874 \text{ atm and } P/\rho RT = 1.0193.$$

According to the Beattie-Bridgman equation,

$$P = 50.2541 \text{ atm and } P/\rho RT = 1.0207.$$

³²White, D., and H. L. Johnston, "The Thermodynamic Properties of Gaseous Hydrogen from Experimental Data of State," AD-27622, November 30, 1953.

(For the same temperature and density, Woolley et al.³¹ give

$$P = 50.2261 \text{ atm and } P/\rho RT = 1.0201.)$$

The densities at 50 atm predicted by the White-Johnston and Beattie-Bridgman equations agree to within 0.1% in the range 100-300°K. Above 300°K, the use of the White-Johnston equation as a standard of comparison is questionable, for the experimental data upon which the equation is based were determined only up to that temperature. A comparison of the Beattie-Bridgman density at 50 atm and 500°K with that determined from the smoothed PVT data reported by Woolley et al.,³¹ also gives agreement to within 0.1%. It is believed that such accuracy is sufficient justification for the use of the Beattie-Bridgman equation as the equation of state for normal hydrogen in the specified range of temperature and pressure.

The thermodynamic properties of para hydrogen up to 300°K appear in tabular form in the literature;³³ these tabulations give the density of para hydrogen at 100°K and 50 atm as 6.046 moles/liter. The corresponding value for normal hydrogen predicted by both the White-Johnston and Beattie-Bridgman equations is 6.053 moles/liter. With this close agreement, and lacking further experimental data on para hydrogen, the PVT properties of ortho and para hydrogen are assumed to be identical.

At temperatures of 1500°K and higher, normal hydrogen is assumed to follow the perfect gas law. Since no experimental PVT data for hydrogen are available at temperatures as high as 1500°K, it is possible only to compare the density at 1500°K and 50 atm with that predicted by the perfect gas law. These are, respectively, 0.4030 and 0.4062 mole/liter. The deviation between these is 0.79%. The effect of dissociation upon density in this temperature range is treated by modifying the perfect gas law to

$$P/\rho RT = 1 + X \quad .$$

In the proposed FORTRAN subroutine, the temperature interval 100-3000°K is divided into three subintervals, 100-600°K, 600-1500°K, and 1500-3000°K; the assumptions stated earlier are used to derive the equations for the thermodynamic properties of hydrogen. In the interval 100-600°K it is assumed that the para composition of the hydrogen remains fixed and that the Beattie-Bridgman equation with the normal constants describes the PVT properties of the real gas, regardless of ortho-para composition. At 600°K, the gas is assumed to convert to the normal composition. In the interval 600-1500°K the gas consists of normal hydrogen, which is again assumed to obey the Beattie-Bridgman equation. At temperatures of 1500-3000°K, the diatomic gas is assumed to be perfect, but dissociation is taken into account.

³³Roden, H., and R. D. Goodwin, Extended Tables of Provisional Thermodynamic Functions for Para Hydrogen, NBS Report 7216 (Dec 14, 1961).

The use of the Beattie-Bridgman equation in evaluating the enthalpy and entropy of normal gaseous hydrogen is discussed in the literature.³⁴ The equations for the enthalpy and entropy are

$$h = h^0 + \left(2\beta - T \frac{d\beta}{dT} \right) \rho + \left(3\gamma - T \frac{d\gamma}{dT} \right) \frac{\rho^2}{2} + \left(4\delta - T \frac{d\delta}{dT} \right) \frac{\rho^3}{3}$$

and

$$S = S' - R' \ln (\rho RT) - \rho \frac{dB}{dT} - \frac{\rho^2}{2} \frac{d\gamma}{dT} - \frac{\rho^3}{3} \frac{d\delta}{dT} \quad .$$

It is seen that the enthalpy of the real gas is equal to that of the ideal gas plus a PVT correction for intermolecular attraction, as determined here from the Beattie-Bridgman equation. The enthalpy of the ideal gas is computed from statistical mechanical principles based on data of the molecular spectra. Similar statements apply to the entropy.

In the interval 100-600°K, the para composition ϕ is held constant. Then,

$$h^0(T) = 526.837\phi + 836.277(1-\phi) + \int_{100}^T [\phi C_p^0 + (1-\phi)C_o^0] dT' \quad .$$

Here 526.837 cal/mole is the enthalpy of ideal para hydrogen at 100°K, and 836.277 cal/mole is the corresponding value for ideal ortho hydrogen.³¹ The functions C_p^0 and C_o^0 are expressed as polynomial expansions in temperature, as shown later. The corresponding entropy is

$$S^0(T) = 23.014\phi + 27.029(1-\phi) + \int_{100}^T \frac{[\phi C_p^0 + (1-\phi)C_o^0] dT'}{T'} \\ + R' \left[\phi \ln \frac{1}{\phi} + (1-\phi) \ln \frac{1}{1-\phi} \right] \quad .$$

Here 23.014 cal/(mole)(°K) is the entropy of ideal para hydrogen and 27.029 cal/(mole)(°K) is the corresponding entropy for ideal ortho hydrogen. The last term in the above equation is the entropy of mixing of the two components. It should be noted that due to the conversion at 600°K, there is a discontinuity in the entropy at this temperature.

Consider, next, the interval 600-1500°K, in which the enthalpy of the ideal normal gas is given by

$$h^0 = 4129.48 + \int_{600}^T C_n^0 dT' \quad ,$$

³⁴McMahon, H., and G. Golden, Calculation of Parameters for Low Pressure Gas Liquefaction Cycles, AECU-3558 (March 1, 1953).

where 4129.48 cal/mole is the enthalpy at 600°K. The entropy is evaluated by going through the following hypothetical steps:

1. The gas of composition ϕ at 600°K is separated into its components, reducing the entropy by

$$R' \left[\phi \ln \frac{1}{\phi} + (1 - \phi) \ln \frac{1}{1 - \phi} \right] .$$

2. At this temperature, the composition is changed to the normal value; since the heat of conversion is essentially zero at this temperature,³¹ ($h_p^0 = 4129.48$ cal/mole; $h_o^0 = 4129.52$ cal/mole), the change of entropy associated with this conversion is negligible.

3. The components at 600°K are mixed, giving an entropy increase of

$$1.98726 \left[0.25 \ln \frac{1}{0.25} + 0.75 \ln \frac{1}{0.75} \right] = 1.118 \text{ eu} .$$

Thus, the entropy of the ideal gas is

$$S^0 = 36.083\phi + 38.266(1 - \phi) + 1.118 + \int_{600}^T \frac{C_n^0 dT'}{T'} .$$

In the interval 1500-3000°K, the diatomic gas is assumed to be ideal, but dissociation must be considered. To do this, an expression for the variation of the heat of dissociation with temperature is developed. The heat of dissociation is given by³¹

$$\Delta H_d^0 = \Delta E_o^0 + 5R'T - h^0 .$$

Here, $\Delta E_o^0 = 103,240$ cal/mole. The variation of $(5R'T - h^0)$ with temperature is shown in Table V-2.

Table V-2

VARIATION OF $(5R'T - h^0)$ WITH TEMPERATURE

T, °K	$5R'T$, cal/mole	h^0 , cal/mole	$(5R'T - h^0)$, cal/mole
1500	14904.5	10697.2	4207.3
2000	19872.6	14679.2	5193.4
3000	29808.9	23230.9	6578.0

These data were fitted to a quadratic equation of the form

$$(5R'T - h^0) = a + bT + cT^2$$

to give

$$\Delta H_d^0 = 103,314 + 3.3432T - 3.9173 \times 10^{-4}T^2 \quad .$$

This result was used in the equation

$$\frac{d \ln K}{dT} = \frac{\Delta H_d^0}{R'T^2} \quad ,$$

subject to the condition that $K = 2.641 \times 10^{-6}$ atm at $2000^\circ K$,³¹ to yield

$$K = 2.641 \times 10^{-6} \exp \left\{ 5.19882 \times 10^4 \left(5 \times 10^{-4} - \frac{1}{T} \right) + 1.68232 \ln \frac{T}{2000} - 1.9712 \times 10^{-4} (T-2000) \right\} \quad .$$

The above equation is used in

$$X = \sqrt{\frac{K}{4P + K}}$$

to solve for the degree of dissociation as a function of temperature and pressure. The enthalpy of the ideal gas (which now depends upon pressure as well as temperature) is computed by taking the normal gas at $1500^\circ K$, heating it to the desired temperature, and then causing dissociation to take place at that temperature

$$h^0(T, P) = 10,697.20 + \int_{1500}^T C_n^0 dT' + X(T) \cdot \Delta H_d^0(T) \quad ,$$

where, 10697.20 cal/mole is the enthalpy of ideal normal hydrogen at $1500^\circ K$. The corresponding entropy is given by

$$\begin{aligned} S^0(T, P) = S^0(1500) - R' \ln P + \int_{1500}^T \frac{C_n^0 dT'}{T'} + \frac{X(T) \cdot \Delta H_d^0(T)}{T} \\ + R' \left[\left(\frac{1-X}{1+X} \right) \ln \left(\frac{1+X}{1-X} \right) + \left(\frac{2X}{1+X} \right) \ln \left(\frac{1+X}{2X} \right) \right] \quad . \end{aligned}$$

In the above equation, the first term on the right-hand side is computed by means of the equation for the ideal entropy in the interval 600 - $1500^\circ K$; the second term corrects for the pressure effect upon the entropy; the fourth term accounts for the entropy increase due to the heat of dissociation; the

last term is the entropy increase due to mixing the monatomic and diatomic species. Then, since the gas is assumed to be ideal,

$$h = h^0 \quad ; \quad S = S^0 \quad .$$

The enthalpy and entropy were expressed in closed form by fitting polynomials in T to values of C^0 reported in the literature. These polynomials included negative powers of T . The C^0 values fitted came from Ref. 31 and 35, except for some of the data for para- H_2 from 100-300°K, which were taken from a more recent report.³⁶ The fits were carefully checked for smoothness and absence of spurious fluctuations between data points. Note that the 600-3000°K range has to be treated in two parts, as does the 100-600°K range for para- H_2 .

The polynomials finally chosen are given below for C^0 in cal/(mole)(°K)

Case 1. Normal H_2 , $1500 \leq T \leq 3000^\circ K$

$$C_n^0 = 5.724193 + 0.1616127 \times 10^{-2}T - 0.1903749 \times 10^{-6}T^2 \quad .$$

The quality of this fit is shown in Table V-3. Here the reported values come from Ref. 35.

Table V-3

SPECIFIC HEAT OF NORMAL HYDROGEN VS
TEMPERATURE FOR $1500 \leq T \leq 3000^\circ K$

T, °K	C_p^0 Calculated, cal/(mole)(°K)	C_p^0 Reported, cal/(mole)(°K)	T, °K	C_p^0 Calculated, cal/(mole)(°K)	C_p^0 Reported, cal/(mole)(°K)
1500	7.7200	7.720	2300	8.4342	8.434
1600	7.8226	7.823	2400	8.5063	8.506
1700	7.9214	7.921	2500	8.5747	8.575
1800	8.0164	8.016	2600	8.6392	8.639
1900	8.1076	8.108	2700	8.6999	8.700
2000	8.1949	8.195	2800	8.7568	8.757
2100	8.2785	8.279	2900	8.8099	8.810
2200	8.3583	8.358	3000	8.8592	8.859

³⁵JANAF Interim Thermochemical Tables, Vol. 2 (Dec 31, 1960).

³⁶Twentieth Bi-monthly Progress Report on the Thermostatic and Transfer Properties of Hydrogen, May 1, 1961 to July 1, 1961, NBS Report 6788.

Case 2. Normal H₂, 600 ≤ T ≤ 1500°K

$$C_n^0 = \frac{0.3401700 \times 10^{12}}{T^4} - \frac{0.1522535 \times 10^{10}}{T^3} + \frac{0.2064732 \times 10^7}{T^2} \\ + \frac{0.4653687 \times 10^3}{T} + 2.954321 + 0.4032975 \times 10^{-2}T \\ - 0.1441460 \times 10^{-5}T^2 + 0.3345081 \times 10^{-9}T^3$$

The data reported in Table V-4 are also from Ref. 35.

Table V-4

SPECIFIC HEAT OF NORMAL HYDROGEN VS
TEMPERATURE FOR 600 ≤ T ≤ 1500°K

T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)	T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)
600	7.0090	7.009	1100	7.2996	7.300
700	7.0360	7.036	1200	7.3900	7.390
800	7.0869	7.087	1300	7.4901	7.490
900	7.1482	7.148	1400	7.6000	7.600
1000	7.2191	7.219	1500	7.7199	7.720

Case 3. Ortho H₂, 100 ≤ T ≤ 600°K

$$C_o^0 = - \frac{0.3154385 \times 10^{15}}{T^7} + \frac{0.3442540 \times 10^{14}}{T^6} - \frac{0.6273164 \times 10^{12}}{T^5} \\ + \frac{0.1050763 \times 10^9}{T^4} + \frac{0.7764858 \times 10^8}{T^3} - \frac{0.4878101 \times 10^6}{T^2} \\ - \frac{0.1528152 \times 10^4}{T} + 0.2765527 \times 10^{+2} - 0.6660184 \times 10^{-1}T \\ + 0.9143383 \times 10^{-4}T^2 - 0.4653937 \times 10^{-7}T^3$$

Data reported in Table V-5 here are from Ref. 31.

Table V-5

SPECIFIC HEAT OF ORTHO HYDROGEN VS
TEMPERATURE FOR 100 ≤ T ≤ 600°K

T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)	T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)
100	5.0391	5.039	300	6.8097	6.809
120	5.1695	5.170	350	6.9185	6.917
150	5.4883	5.487	400	6.9605	6.963
200	6.1086	6.110	500	6.9928	6.992
250	6.5646	6.565	600	7.0088	7.009

Since the C_p^0 for para H_2 has a maximum at $T = 170^\circ K$, it was found convenient to split the 100-600-degree region in two at that point.

Case 4. Para H_2 , $170 \leq T \leq 600^\circ K$

$$C_p^0 = \frac{0.2247810 \times 10^{17}}{T^7} - \frac{0.2425375 \times 10^{15}}{T^6} + \frac{0.1554964 \times 10^{12}}{T^5} \\ + \frac{0.1185768 \times 10^{10}}{T^4} + \frac{0.2340575 \times 10^8}{T^3} - \frac{0.1164820 \times 10^6}{T^2} \\ + \frac{0.1144968 \times 10^4}{T} + 0.2411355 + 0.1400111 \times 10^{-1}T \\ - 0.1322382 \times 10^{-5}T^2 - 0.2673443 \times 10^{-7}T^3 + 0.2252643 \times 10^{-10}T^4$$

The data reported in Table V-6 above $300^\circ K$ are from Ref. 31, whereas the data at $300^\circ K$ and below are from Ref. 36 and have been multiplied by $R' = 1.98726 \text{ cal}/(\text{mole})(^\circ K)$ to bring them into agreement with the system of units used here.

Table V-6

SPECIFIC HEAT OF PARA HYDROGEN VS
TEMPERATURE FOR $170 \leq T \leq 600^\circ K$

T, $^\circ K$	C_p^0 Calculated, cal/(mole)($^\circ K$)	C_p^0 Reported, cal/(mole)($^\circ K$)
170	7.883891	7.88376
180	7.858525	7.85894
190	7.808729	7.80848
200	7.742622	7.74227
210	7.668112	7.66802
220	7.591267	7.59143
230	7.516233	7.51647
240	7.445593	7.44575
250	7.380793	7.38080
260	7.322486	7.32234
270	7.270807	7.27059
280	7.225566	7.22540
290	7.186377	7.18633
300	7.152747	7.15292
350	7.049324	7.049
400	7.011804	7.010
500	6.999750	6.998
600	7.010365	7.010

Case 5. Para H₂, 100 ≤ T ≤ 170°K

$$C_p^0 = \frac{0.9285017 \times 10^7}{T^3} - \frac{0.2340802 \times 10^6}{T^2} + \frac{0.1773508 \times 10^4}{T} \\ - 1.619946 + 0.4490101 \times 10^{-1}T + 0.2250453 \times 10^{-3}T^2 \\ - 0.2956882 \times 10^{-5}T^3 + 0.6790110 \times 10^{-8}T^4$$

The data reported in Table V-7 are from Ref. 36 and have been treated as described above.

Table V-7

SPECIFIC HEAT OF PARA HYDROGEN VS
TEMPERATURE FOR 100 ≤ T ≤ 170°K

T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)	T, °K	C _p ⁰ Calculated, cal/(mole)(°K)	C _p ⁰ Reported, cal/(mole)(°K)
100	6.454814	6.45462	140	7.680687	7.68118
110	6.854043	6.85480	150	7.807679	7.80785
120	7.204270	7.20346	160	7.871470	7.87110
130	7.481199	7.48102	170	7.883668	7.88376

Tables V-8, V-9, and V-10 show comparisons between values of ideal entropy and enthalpy calculated by a modification of this subroutine and values reported in Table 4 of Ref. 31. The tables are for ortho, para, and normal hydrogen at one atmosphere. Note that the entropy values at

Table V-8

ENTHALPY AND ENTROPY FOR ORTHO HYDROGEN

T, °K	Enthalpy, cal/(mole)(°K)		Entropy, eu	
	Calculated	Reported	Calculated	Reported
100	836.284	836.277	27.029	27.029
120	938.089	938.227	27.956	27.959
150	1097.72	1097.78	29.142	29.143
200	1387.82	1387.90	30.807	30.808
250	1705.61	1705.80	32.224	32.225
300	2040.71	2040.87	33.445	33.446
350	2384.32	2384.39	34.504	34.505
400	2731.46	2731.54	35.431	35.432
500	3429.28	3429.53	36.988	36.990
600	4129.48	4129.52	39.383*	38.266
700	4831.38	4831.66	40.465*	39.348
1000			43.003*	41.884
1500			46.022*†	44.903
2000			48.377*†	47.190

*Includes entropy of mixing due to conversion to normal at 600°K

†Includes effect of dissociation at one atmosphere

Table V-9

ENTHALPY AND ENTROPY FOR PARA HYDROGEN

T, °K	Enthalpy, cal/(mole)(°K)		Entropy, eu	
	Calculated	Reported	Calculated	Reported
100	526.839	526.837	23.014	23.014
120	663.752	663.752	24.260	24.259
150	890.615	890.605	25.945	25.945
200	1282.73	1282.70	28.202	28.202
250	1660.55	1660.49	29.889	29.889
300	2023.25	2023.16	31.213	31.212
350	2377.91	2377.84	32.306	32.306
400	2729.26	2729.19	33.245	33.244
500	3429.55	3429.24	34.807	34.806
600	4129.48	4129.48	37.200*	36.083
700	4831.38	4831.65	38.282*	37.165
1000			40.820*	39.701
1500			43.839*†	42.720
2000			46.194*†	45.007

*Includes entropy of mixing due to conversion to normal at 600°K

†Includes effect of dissociation at one atmosphere

Table V-10

ENTHALPY AND ENTROPY FOR NORMAL HYDROGEN

T, °K	Enthalpy, cal/(mole)(°K)		Entropy, eu	
	Calculated	Reported	Calculated	Reported
100	758.923	758.916	27.142	27.142
120	869.505	869.609	28.150	28.151
150	1045.95	1045.99	29.460	29.461
200	1361.55	1361.61	31.273	31.275
250	1694.35	1694.47	32.757	32.758
300	2036.35	2036.44	34.004	34.005
350	2382.72	2382.75	35.072	35.073
400	2730.91	2730.95	36.002	36.003
500	3429.35	3429.46	37.560	37.561
600	4129.48	4129.51	38.838	38.838
700	4831.38	4831.66	39.920	39.920
1000	6967.38	6966.23	42.457	42.455
1500	10698.11*	10697.20	45.476*	45.475
2000	14767.98*	14679.2	47.831*	47.762
3000	31868.76*	23230.9	54.926*	51.221

*Includes effect of dissociation at one atmosphere

600°K and above for ortho and para hydrogen include an entropy-of-mixing term of 1.1175 eu, since conversion to normal at 600°K is assumed. Also, all quantities above 1500°K include the effect of dissociation at one atmosphere. With these exceptions, the calculated and reported values agree to four significant figures, except for a few isolated enthalpy values which are off by no more than one in the fourth figure.

To check the Beattie-Bridgman calculations, a number of cases were calculated and compared with data tabulated in Ref. 34. The results are shown in Table V-11. Note that there are only occasional discrepancies of as much as one in the fourth significant figure in density and entropy and in the fifth significant figure in enthalpy.

Table V-11

BEATTIE-BRIDGMAN CALCULATIONS

		T(°K) =	100	150	200	250	300
P = 1 atm							
Enthalpy, cal/(mole)(°K):	calculated		758.2	1045.7	1361.5	1694.4	2036.5
	reported		758.2	1045.7	1361.5	1694.5	2036.6
Entropy, eu:	calculated		27.14	29.46	31.27	32.76	34.00
	reported		27.14	29.46	31.27	32.76	34.00
Density, moles/liter:	calculated		0.1219	0.08122	0.06090	0.04872	0.04060
	reported		0.1219	0.08121	0.06090	0.04872	0.04060
P = 4 atm							
Enthalpy, cal/(mole)(°K):	calculated		756.1	1044.8	1361.2	1694.5	2036.8
	reported		756.1	1044.9	1361.3	1694.6	2036.9
Entropy, eu:	calculated		24.36	26.70	28.51	30.00	31.25
	reported		24.36	26.70	28.51	30.00	31.25
Density, moles/liter:	calculated		0.4883	0.3245	0.2432	0.1946	0.1622
	reported		0.4882	0.3244	0.2432	0.1945	0.1621
P = 16 atm							
Enthalpy, cal/(mole)(°K):	calculated		748.1	1041.8	1360.6	1695.2	2038.4
	reported		748.1	1041.9	1360.6	1695.3	2038.5
Entropy, eu:	calculated		21.54	23.91	25.74	27.23	28.48
	reported		21.54	23.91	25.74	27.23	28.49
Density, moles/liter:	calculated		1.958	1.290	0.9659	0.7728	0.6444
	reported		1.958	1.290	0.9659	0.7728	0.6443

The subroutine (see Table V-12) is called by a FORTRAN statement of the form CALL STATE (T, P, PHI, RH ϕ , H, S, X) where the arguments are as follows:

Input arguments: T = temperature, °K
P = pressure, atm
PHI = fraction para (= 0.25 for normal hydrogen)

Output arguments: RH ϕ = density, moles/liter
H = enthalpy, cal/mole
S = entropy, cal/mole
X = fraction dissociated

The subroutine uses 927 memory locations plus space for the LOG, EXP, and SQRT routines when compiled for the IBM-704.

Table V-12

FORTRAN--II SUBROUTINE FOR HYDROGEN PROPERTIES

```

SUBROUTINE DENS (TEMP, PRESS, PARA, DENALP, TROP, DISS, )
T=TEMP
P=PRESS
PHI=PARA
TL=LOGF(T)
ALPHA=.082060*T
RHO=P/ALPHA
IF(T-1500.)2,1,1
1 X=2.641E-6*EXP(5.19882E4*(5.E-4-1./T)+1.68232*LOGF(T/2000.))
1-1.9712E-4*(T-2000.))
X=SQRTF(X/(4.*P+X))
H=506.9+X*(103314.+T*(3.3432-T*3.9173E-4))
1+T*(5.724193+T*(.8080635E-3-T*.634583E-7))
S=1.9482-2.183*PHI-1.98726*LOGF(P)+X*(103314./T+3.3432-3.9173E-4*T
1)+1.98726*((1.-X)/(1.+X))*LOGF((1.+X)/(1.-X))+((2.*X/(1.+X))*LOGF
2((1.+X)/(2.*X)))+5.724193*TL+T*(.1616127E-2-T*.9518745E-7)
RHO=RHO/(1.0+X)
GOTO3
2 X=0.
T2=T**2
T3=T2*T
BETA=.02096*ALPHA-.1975-41.358240/T2
GAMMA=.9136464E-3*ALPHA-.99935E-3-.86686871/T2
DELTA=-.037786807/T2
5 PREV=RHO
RHO=(P-RHO**2*(BETA+RHO*(GAMMA+RHO*DELTA)))/ALPHA
IF(ABSF(RHO-PREV)/RHO-1.E-5)4,4,5
4 RHU=RHO*24.21716
H=RHU*(2.*BETA-.02096*ALPHA-82.716480/T2+RHO*(1.5*GAMMA-
1.3748691E-4*T-.86686871/T2+RHO*2.0*DELTA))
S=-1.98726*LOGF(RHO*ALPHA)-RHU*(.1719978E-2+82.716480/T3
1+RHO*(.3748691E-4+.86686871/T3+RHO*.66666667*DELTA/T))
IF(T-600.)7,6,6
6 H=H+600.13-(.11339E12-T*(.7612675E9-T*.2064732E7))/T3
1+.4653687E3*TL+T*(2.954321+T*(.2011988E-2
2+T*(-.4804867E-6+T*.8362703E-10)))
S=S+20.2558-2.183*PHI-(.850425E11+T*(-.5075117E9
1+T*(.1032366E7+T*.4653687E3))/T2**2+2.954321*TL
2+T*(.4023975E-2-T*(.72073E-6-T*.1115027E-9))
GOTO3
7 T6=T3**2
H=H+3518.842-2992.005*PHI+(1.0-PHI)*(-(.5258058E14
1+T*(.688508E13+T*(-.1568291E12+T*(.3502543E8+T*(.3882429E8
2-T*.4878101E6)))))/T6-.1528152E4*TL+T*(.2765527E+2
3+T*(-.3330092E-1+T*(.3047794E-4-T*.1163484E-7))))
T7=T6*T
S=S-114.896+137.91*PHI+(1.0-PHI)*(-(.4506264E14
1+T*(.5737567E13+T*(-.1254633E12+T*(.2626908E8
2+T*(.2588286E8+T*(-.2439051E6-T*.1528152E4)))))/T7
3+.2765527E+2*TL+T*(-.6660184E-1+T*(.4571692E-4-T*.1551312E-7)))
4-1.98726*(PHI*LOGF(PHI)+(1.0-PHI)*LOGF(1.0-PHI))
IF(T-170.)9,8,8
8 H=H+PHI*(-5935.1644-(.374635E16+T*(-.485075E14
1+T*(.388471E11+T*(.395256E9+T*(.1170288E8-T*.116482E6)))))/T6
2+.1144968E4*TL+T*(.2411355+T*(.7000555E-2+T*(-.440794E-6
3-T*(.6683608E-8-T*.4505286E-11))))
S=S+PHI*(6.344314-(.3211157E16+T*(-.4042292E14
1+T*(.3109928E11+T*(.296442E9+T*(.7801917E7+T*(-.58241E5
2+T*.1144968E4)))))/T7+.2411355*TL+T*(.1400111E-1
3+T*(-.661191E-6-T*(.8911477E-8-T*.5631608E-11))))
GOTO3
9 H=H+PHI*(-10121.039-(.4642509E7+T*(-.2340802E6))/T2
1+.1773508E4*TL+T*(-1.619946+T*(.2245051E-1
2+T*(.750151E-4+T*(-.7392205E-6+T*.1358022E-8))))
S=S+PHI*(11.786749-(.3095006E7+T*(-.1170401E6
1+T*.1773508E4))/T3-1.619946*TL+T*(.4490101E-1
2+T*(.1125227E-3+T*(-.9856273E-6+T*.1697528E-8))))
3 DENS=RHO
THALP=H
TROP=S
DISS=X
RETURN

```


VI. CONSIDERATIONS PERTAINING TO REACTOR KINETICS AND CONTROL

David Sparks

A. Influence of "Period Effect" Phenomena on Design of Nuclear Rocket Systems

The period effect^{37,38} is of potentially vital importance to the design of nuclear rocket reactor systems. The effect tends to decrease stability in a reactor system when it is on a rising period shorter than about 30 sec. Since periods shorter than this will be required and good stability of the system is mandatory, it is apparent that any proposed system must be carefully evaluated with regard to the influence of the period effect.

It is probable that the temperature of core materials will be the limiting factor in system design. For this reason, direct servo control of the reactor based on such temperatures may be desirable, providing stability of the servo system can be achieved with the loop closed on temperature. Closed-loop control of temperature will, in general, be more difficult (than power, for instance) as regards stability due to thermal time lags, which are in series with the main control loop. This fact, and also the extreme power densities required of the system, make it entirely possible that stability could become a limiting factor in the reactor design; thus, the destabilizing influence of the period effect would be of prime importance.

It might appear at first inspection of the Bode plots for the period equilibrium transfer function given in Ref. 38 that the destabilizing influence of the period effect in terms of increased gain and phase lag might be more serious for systems of shorter neutron lifetimes. However, this is not the case. It is pointed out in Ref. 37 that the period equilibrium transfer function (whose Bode plots are given in Ref. 38) is not the correct function by which to represent the reactor in stability studies. The correct function is the ILES transfer function which is presented in Ref. 37. Figures VI-1 and VI-2 show the comparison between the Bode plots for these two transfer functions. It should be noted that the curves of the period equilibrium transfer function appear to become independent of period as period becomes less than about 0.1 sec in the case presented, for which $l^* = 10^{-3}$ sec. The gain curve tends to approach the $1/S1^*$ asymptote and the phase approaches -90° . This would tend to indicate that

³⁷Carter, J. C., D. W. Sparks, and J. H. Tessier. The Period Effect in Reactor Dynamics, Presented at the Symposium on Reactor Kinetics and Control, University of Arizona, Tucson, March 25, 1963.

³⁸Singer, Sidney. The Period Equilibrium Effect in Reactor Dynamics, LA-2654 (March 1962).

further changes in gain and phase would not occur for periods below 0.1 sec in this case. Since these asymptotic limits are approached at larger periods for smaller ℓ^* , one is led, incorrectly, to assume that, for a given period, large ℓ^* would be advantageous from the standpoint of period effects. It can be seen from the figures that for the ILES transfer function, which is the correct representation of the reactor, neither the phase nor the amplitude approaches a fixed curve as period approaches zero.

Fig. VI-1. Comparison of ILES and Period Equilibrium Transfer Function Bode Plots - Gain.

Fig. VI-2. Comparison of ILES and Period Equilibrium Transfer Function Bode Plots - Phase.

From the tables of values of the poles of the ILES transfer function given in Appendix C of Ref. 37, it appears that ℓ^* has little influence on the relative susceptibility of a reactor system to the destabilizing effects of a positive period. As can be seen from the tables, the position of the pole, p_1 , (which for positive period is in the right half s -plane) continues to be a function of k'_{ex} regardless of ℓ^* . It is the motion of this pole which is the primary contributing factor to the destabilizing influence of period. In addition, as k'_{ex} approaches prompt critical, the pole, p_1 (which for large periods is so remote in the left half plane that its influence on stability is negligible) moves to a value near that of the other poles and thus adds a further destabilizing influence. This pole will have little or no influence on stability until it has become > -100 rad/sec for rocket reactor control systems. It can be seen from the tables of Appendix C, Ref. 37 that this occurs at smaller values of k'_{ex} (hence longer period) for large ℓ^* systems. From this standpoint, then, one might argue that the period effect is more serious in large ℓ^* systems. In actual fact, however, the influence of period effect on stability of a given system is so intricately tied in with the dynamic characteristics of the individual system that no such general statements can properly be made based only on the ℓ^* of the system.

The most correct general statement concerning ℓ^* alone is the statement previously made that ℓ^* has little influence on the relative susceptibility of a system to the destabilizing influence of positive period. In any case, the period effect will need be accounted for in the control design whenever periods of 30 sec or less are to be experienced. The actual design changes necessary to correct for the period effect may be considerably different for different ℓ^* , but probably not significantly different in difficulty of implementation.

Fig. VI-3. Incremental Linear Equivalent System for the Neutron Kinetics Equations.

It is shown in Ref. 37 that the reactor is correctly represented by the Incremental Linear Equivalent System shown in Fig. VI-3. The ILES transfer function is the transfer function relating the input Δk_{ex} shown in the figure to its corresponding terms in the output. As can be seen, this transfer function is dependent only on k'_{ex} and n' , and not on any other initial conditions. This fact points immediately to the fact that a completely general form of nonlinear compensation network can be designed in which time constants and gain need be adjusted as functions of k'_{ex} and power only. In an actual reactor system, the instanta-

neous measurement of the effective k'_{ex} (including that due to internal feedback) could be obtained from measured power by methods described in Ref. 37.

Through use of this measured value of instantaneous effective k'_{ex} , gain and time constants could be adjusted to compensate for the period effect, thus yielding a reactor servo control system with specified bandwidth or specified accuracy for an arbitrary input or disturbance.

From Fig. VI-3 it may be seen that for the range of frequency above which the gain of the feedback function shown in the figure has become negligible, the ILES transfer function becomes essentially equal to the forward transfer function shown, i.e.,

$$\left. \frac{\Delta n / n'}{\Delta k_{ex}} \right]_{\omega > 10} \approx \frac{1 / \ell^*}{s + (1 / \ell^*) [\beta - k_{ex} (1 - \beta)]} .$$

Thus, in the frequency range in which the significant dynamics of nuclear rocket reactor control systems will lie, the reactor is approximately represented by a first-order system with a steady-state gain of $1/[\beta - k'_{ex}(1 - \beta)]$ and a corner frequency of $1/\ell^* [\beta - k'_{ex}(1 - \beta)]$. For reactor systems in which this corner frequency is beyond the desired control system bandwidth for any desired period, it is quite likely that the only nonlinearity needed in the compensation network will consist of a gain correction proportional to $[\beta - k'_{ex}(1 - \beta)]$ in series with the main servo control loop. For systems with large ℓ^* , the above corner frequency, which is a function of k'_{ex} , likely will lie in the region of gain crossover of the control loop, and hence may necessitate more complex nonlinear compensation to counteract period effects.

B. Bandwidth Considerations in Design of Nuclear Rocket Reactor Systems

As mentioned above, it seems quite likely that it will be desirable to control reactor power to maintain structural temperature constant. Rocket thrust would then be controlled by varying propellant flow rate. The reactor servo control system would be designed to maintain core structural temperature constant while propellant flow varies from zero to maximum. Such a system would appear very desirable in that propellant outlet temperature (and hence specific impulse) would be maintained approximately constant at its maximum value consistent with structural temperature limits. At the same time, thermal shock on structural materials would be minimized.

In order for the reactor control system actually to maintain constant temperature while propellant flow is being rapidly changed from zero to full flow will require a very "stiff" or wide bandwidth servo system. It is difficult to specify at present what bandwidth will be required, but it is safe to say that it will probably lie in the range from 1 to 10 cps or higher, depending on the spectrum of noise inherent in the propellant flow, and the time constants of the fuel elements or other critical core structural members.

In regard to reactor servo control system bandwidth, the influence of neutron lifetime becomes of great importance. Systems with large ℓ^* have less inherent bandwidth, and so may become a serious limiting factor in a design in which wide bandwidth is important.

Although a system with large ℓ^* can in principle be designed so as to have any desired bandwidth of the closed loop, it will require higher gain in the control actuators than would a reactor with smaller ℓ^* for the same control response. Since the reactor with larger ℓ^* has a lower gain, this must be compensated by higher gain in the control loop.

This higher actuator gain exacts no serious penalty on the system where external disturbances which are manifested only as reactivity changes are concerned. However, if the disturbance results from the change of

thermal load due to changes of propellant flow rate, the actuator motions required of the reactor control system may become prohibitively large if system bandwidth beyond the β/ℓ^* high-frequency roll-off of the reactor is required. For example, assume that a 3-cps bandwidth is desirable. For $\ell^* = 5 \times 10^{-4}$ sec, an actuator gain roughly twice that of a 10^{-5} -sec system is required. This means that for equal stabilization against reactor temperature disturbances caused by flow variations at 3 cps, the magnitude of actuator reactivity changes required in the former system would be twice as great as in the 10^{-5} -sec system.

Thus, the bandwidth advantage of a short ℓ^* would be the principal reason for its choice if servo control characteristics were the only criterion. The chief disadvantage of a system with short ℓ^* is, of course, its capability for more rapid excursion in case of a catastrophic accidental reactivity insertion.

That this capability represents a disadvantage over a system with larger ℓ^* is, after all, based on the assumption that in the system with large ℓ^* the excursion would be slower so that there would be a better chance of counteracting it by control actuator movement. Although this assumption may possibly be true to some extent, it will certainly be dangerous to depend on actuator movement alone in any reactor. In other words, it would seem mandatory, regardless of lifetime, to design any core to have internal temperature feedback capable of limiting the maximum credible accident as required.

Hence, this seeming disadvantage of a system with short ℓ^* is only academic if either system can be designed with internal feedback capable of limiting a specified reactivity accident to a specified release of energy. It makes little difference whether the energy was released in a few microseconds or a few milliseconds.

VII. THERMAL STRESSES IN REACTOR FUEL PLATES

I. The Plane Strain Elasticity Solution

C. K. Youngdahl

One of the concepts that has been considered is the use of parallel, flat-plate fuel assemblies in reactor cores. Under high-temperature operating conditions, the long-term response of the plates to thermal and mechanical loading would be strongly time dependent and, hence, a visco-elastic analysis would be appropriate. However, during startup or fluctuations in operating conditions, the immediate response would be elastic in nature, and ordinary linear elasticity theory should give an accurate determination of the stresses and displacements. The first part of this article gives the exact thermo-elasticity solution for arbitrary temperature distribution and normal surface tractions; the second part gives some thin-plate approximations to this solution.

A. Exact Solution

1. Introduction

The thermal stresses and displacements corresponding to an arbitrary temperature distribution in a fuel plate are determined here using linear thermo-elasticity theory. The temperature distribution may be given in the form of an analytical or numerical solution to a theoretical problem or may be derived from experimental measurements, the only restriction being that the distribution possess a Fourier series expansion. The associated stresses and displacements are found in terms of the coefficients of this expansion.

If the prescribed temperature is independent of time, then the stress field derived here is the equilibrium solution; if the temperature field is time dependent, then this is the corresponding quasistatic elasticity solution, i.e., the inertia term in the equation of motion for the material has been neglected. It is generally accepted that the quasistatic solution is an excellent approximation to the dynamic solution except in some mathematically pathological (and physically implausible) cases.

Stresses due to drag loads of the coolant on the plate and body forces are not included here, as the intent is to study the thermal effect. Due to the assumed linearity of the problem, these stresses may be superimposed later. However, arbitrary normal loading on the plate surfaces is incorporated into the solution since it requires little additional effort to do so.

The elastic constants of the plate material and its coefficient of thermal expansion are assumed to be independent of position and temperature; however, the temperature dependence of the coefficient of thermal expansion may be incorporated into the solution quite easily.

In order to simplify the problem, it is assumed that the temperature and normal surface loading are constant across the width of the plate and that a condition of plane strain exists in this direction. No simplifying assumptions (such as the existence of plane stress, for example) are made about the temperature and stress variations through the thickness of the plate, since, even though the thickness may be very small compared to the other plate dimensions, the temperature and stress variations in this direction may be significant. It seems physically plausible to assume, however, that the temperature and loading are symmetric about the midplane of the plate. These assumptions of plane strain and symmetry considerably simplify the algebra involved in the solution of the thermoelastic problem, but the technique used here could also be applied to an arbitrary three-dimensional temperature variation if it were decided that the added accuracy warranted the necessary algebraic effort.

The expressions for the resultant thermal stresses and displacements are in the form of Fourier series. The coefficients in these series will have to be determined numerically as the solutions to a set of simultaneous linear algebraic equations and will be functions of the coefficients of the Fourier series expansions for the prescribed temperature field and normal loading on the boundary.

2. Statement of Problem

a. Fuel Plate. The plate length, width, and thickness are $2b$, $2c$, and $2a$, respectively, with coolant flow in the y direction, as indicated in the figure. The origin o of the coordinate system is at the geometric center of the plate. The material is assumed to be homogeneous and isotropic, and its shear modulus μ , Poisson's ratio ν , and coefficient of thermal expansion α are independent of the temperature $T(x,y,z,t)$.* The applied body forces are assumed to be zero.

*If α is a function of temperature, replace αT by $\int_0^T \alpha(T) dT$ wherever it appears.

b. Thermo-elastic Field Equations. The temperature distribution and surface loading on the plate produce stresses σ_{xx} , σ_{yy} , σ_{zz} , σ_{xy} , σ_{yz} , σ_{zx} and displacements u_x , u_y , u_z . Since the quasistatic solution will be obtained, the time dependence enters in only through the temperature; hence, t will be treated as a parameter rather than as an independent variable, and an elastic equilibrium formulation is appropriate. The displacement equations of equilibrium for zero body forces are, in indicial notation,*

$$(1 - 2\nu)u_{i,kk} + u_{k,ki} - 2(1 + \nu)\alpha T_i = 0 \quad , \quad (1)$$

and the stress-displacement relations are

$$\sigma_{ij} = \mu \left[u_{i,j} + u_{j,i} + \frac{2\nu}{1 - 2\nu} \delta_{ij} u_{k,k} - \frac{2(1 + \nu)}{1 - 2\nu} \delta_{ij} \alpha T \right] \quad , \quad (2)$$

where δ_{ij} is the Kronecker delta. The three equations represented by (1) and the six equations by (2), along with appropriate boundary conditions, comprise a system of nine partial differential equations in nine dependent variables - three displacements and six stresses - and three independent variables - the space coordinates x , y , z . In order to make this formidable array more tractable, stress functions are commonly introduced. These decrease the number and complexity of the differential equations at the expense of complicating the boundary conditions.

c. Generalized Papkovitch Stress Functions.³⁹ Let the displacement field be given in terms of the generalized Papkovitch stress functions ϕ , ψ_x , ψ_y , ψ_z through

$$u_i = (\phi + x_k \psi_k)_{,i} - 4(1 - \nu)\psi_i \quad . \quad (3)$$

Then the equilibrium equations (1) are equivalent to

$$\phi_{ii} = \frac{1 + \nu}{1 - \nu} \alpha T \quad ; \quad \psi_{i,jj} = 0 \quad . \quad (4)$$

*Subscripts take on the values 1, 2, 3; commas denote differentiation; repeated subscripts are summed over; and the 1, 2, 3 directions correspond to x , y , z , respectively. For example,

$$u_1 = u_x \quad ; \quad \sigma_{23} = \sigma_{yz} \quad , \quad u_{3,kk} = \nabla^2 u_z \quad ; \quad T_1 = \frac{\partial T}{\partial x} \quad .$$

³⁹Sternberg, E. and E. L. McDowell, On the Steady-state Thermoelastic Problem for the Half-space, Quart. Appl. Math., 14, 4, 381 (1957).

Substituting (3) into (2) and making use of (4) gives the stresses in terms of the stress functions, namely,

$$\frac{\sigma_{ij}}{2\mu} = (\phi + x_k \psi_k)_{,jj} - 2(1-\nu)(\psi_{i,j} + \psi_{j,i}) - 2\nu \delta_{ij} \psi_{k,k} - \frac{1+\nu}{1-\nu} \delta_{ij} \alpha T \quad (5)$$

Since, by (4), the ψ_i and the homogeneous part of ϕ are solutions to the thoroughly investigated Laplace's equation, we have greatly simplified the problem of finding general solutions to the field equations. However, the boundary conditions for the displacements and stresses now become, through (3) and (5), differential equations in the stress functions.

There is a theorem⁴⁰ in elasticity theory which says that for convex domains and zero body forces, one of the stress functions ψ_i can be taken equal to zero without loss of generality. Therefore, let

$$\psi_y = 0 \quad (6)$$

d. Prescribed Temperature Distribution. Assume that T is independent of z , that is, the temperature may vary along the length and through the thickness of the plate but not across its width. In addition, let the temperature distribution be symmetric about the plane $x = 0$. Then we have

$$T(x,y,t) = T(-x,y,t) \quad (7)$$

Because of the shape of the fuel plate, it seems reasonable to express T as a double Fourier series in x and y , obtained by applying Fourier analysis techniques to the analytical, numerical, or experimental results for the temperature field. Therefore, keeping (7) in mind, let us assume we are given T in the form*

$$\begin{aligned} \frac{1+\nu}{1-\nu} \alpha T(x,y,t) = & A_0(t) + \sum_m A_{m0}(t) \cos \alpha_m x \\ & + \sum_n [A_{0n}(t) \cos \beta_n y + B_{0n}(t) \sin \beta_n y] \\ & + \sum_m \sum_n \cos \alpha_m x [A_{mn}(t) \cos \beta_n y + B_{mn}(t) \sin \beta_n y] \quad (8) \end{aligned}$$

⁴⁰Eubanks R. A. and E. Sternberg, On the Completeness of the Boussinesq-Papkovich Stress Functions, J. of Ratl. Mech. and Anal., 5, 5, 735 (1956).

*Remember that if α is temperature dependent replace αT by $\int_0^T \alpha dT$.

where

$$\alpha_m = \frac{m\pi}{a} \quad ; \quad \beta_n = \frac{n\pi}{b} \quad ; \quad m,n = 1, 2, 3 \dots \quad , \quad (9)$$

and the A's and B's are dimensionless. The notation $\sum_j$ used here and in subsequent equations means that j is to be summed from 1 to ∞ . In (8), the $\frac{1+\nu}{1-\nu}$ α factor has been included on the left side of the equation for later algebraic convenience.

e. Plane Strain. Since it seems physically reasonable to assume that the boundary loading will be independent of z and since it has been assumed that the temperature distribution is not a function of z either, a plane strain solution looks promising. Plane strain implies that we set*

$$u_z = 0 \quad ; \quad u_x = u_x(x,y) \quad ; \quad u_y = u_y(x,y) \quad , \quad (10)$$

or, equivalently, in terms of the Papkovitch stress functions,**

$$\phi = \phi(x,y) \quad ; \quad \psi_x = \psi_x(x,y) \quad ; \quad \psi_z = 0 \quad . \quad (11)$$

Equations (4) then become

$$\begin{aligned} \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} &= \frac{1+\nu}{1-\nu} \alpha T \quad ; \\ \frac{\partial^2 \psi_x}{\partial x^2} + \frac{\partial^2 \psi_x}{\partial y^2} &= 0 \quad . \end{aligned} \quad (12)$$

Substituting (11) into (3) and (5) gives

$$\left. \begin{aligned} u_x &= \frac{\partial}{\partial x} (\phi + x\psi_x) - 4(1-\nu)\psi_x \quad ; \\ u_y &= \frac{\partial}{\partial y} (\phi + x\psi_x) \quad ; \\ u_z &= 0 \quad ; \end{aligned} \right\} \quad (13)$$

*Since in the quasistatic elastic solution time appears only as a parameter, it will not be written as an independent variable any more.

**Recall that $\psi_y = 0$ by (6).

$$\left. \begin{aligned}
\frac{\sigma_{xx}}{2\mu} &= \frac{\partial^2}{\partial x^2} (\phi + x\psi_x) - 2(2-\nu) \frac{\partial\psi_x}{\partial x} - \frac{1+\nu}{1-\nu} \alpha T \quad ; \\
\frac{\sigma_{yy}}{2\mu} &= \frac{\partial^2}{\partial y^2} (\phi + x\psi_x) - 2\nu \frac{\partial\psi_x}{\partial x} - \frac{1+\nu}{1-\nu} \alpha T \quad ; \\
\frac{\sigma_{zz}}{2\mu} &= -2\nu \frac{\partial\psi_x}{\partial x} - \frac{1+\nu}{1-\nu} \alpha T \quad ; \\
\frac{\sigma_{xy}}{2\mu} &= \frac{\partial^2}{\partial x \partial y} (\phi + x\psi_x) - 2(1-\nu) \frac{\partial\psi_x}{\partial y} \quad ; \\
\sigma_{yz} &= \sigma_{zx} = 0 \quad .
\end{aligned} \right\} \quad (14)$$

f. Boundary Conditions. We will assume that the applied shearing stresses are zero everywhere on the boundary; on the other hand, the normal loading can be quite general provided that the symmetry of the problem about the plane $x = 0$ is maintained. This symmetry implies that

$$\begin{aligned}
\sigma_{xx}(x,y) &= \sigma_{xx}(-x,y) \quad ; \\
\sigma_{yy}(x,y) &= \sigma_{yy}(-x,y) \quad ; \\
\sigma_{xy}(x,y) &= -\sigma_{xy}(-x,y) \quad .
\end{aligned} \quad (15)$$

Let us assume that the non-zero prescribed loading can be expanded in Fourier series and take the boundary conditions on the plate as

$$\frac{\sigma_{xx}(a,y)}{2\mu} = \frac{\sigma_{xx}(-a,y)}{2\mu} = P_1 + \sum_n (P_{1n} \cos \beta_n y + Q_{1n} \sin \beta_n y) \quad ; \quad (16)$$

$$\sigma_{xy}(a,y) = \sigma_{xy}(-a,y) = 0 \quad ; \quad (17)$$

$$\frac{\sigma_{yy}(x,b)}{2\mu} = P_2 + \sum_m P_{2m} \cos \alpha_m x \quad ; \quad (18)$$

$$\frac{\sigma_{yy}(x,-b)}{2\mu} = P_3 + \sum_m P_{3m} \cos \alpha_m x \quad ; \quad (19)$$

$$\sigma_{xy}(x,b) = 0 \quad ; \quad (20)$$

$$\sigma_{xy}(x,-b) = 0 \quad , \quad (21)$$

where α_m , and β_n are given by (9), and the P's and Q's are dimensionless. Overall equilibrium of the plate requires that

$$P_2 = P_3 \quad . \quad (22)$$

Note that, having made the assumption of plane strain, we are no longer free to prescribe the boundary conditions on the surfaces $z = \pm c$. From (13), and (14) we see that $u_z = \sigma_{yz} = \sigma_{zx} = 0$ everywhere in the plate, so that the boundary conditions on the surfaces $z = \pm c$ must be zero normal displacement and zero shearing load. Taking the stress functions in the form (11) assures that these conditions are met.

g. Resultant Statement of Problem. The system of partial differential equations to be solved is (12) with T given by (8). The boundary conditions on these equations are given by combining (14) with (16)-(21).

3. Construction of the Stress Functions

a. Construction of ψ_x . By means of the technique of separation of variables, it is easy to show that polynomials of the form $k_0 + k_1x + k_2y + k_3xy$ and exponentials of the form $(k_4e^{\gamma x} + k_5e^{-\gamma x})(k_6e^{i\gamma y} + k_7e^{-i\gamma y})$, where γ may be real or imaginary, are solutions of the second of (12).^{*} Because of the symmetry of the problem about the plane $x = 0$, the stress function ψ_x must be an odd function of x . Inspection of the forms of the Fourier series for the temperature distribution and the boundary conditions given by (8) and (16)-(21), respectively, leads us to take ψ_x as

$$\begin{aligned} \psi_x = & \frac{1}{2}C_1x + \sum_m \alpha_m^{-1} \sin \alpha_m x (C_{1m} \cosh \alpha_m y + S_{1m} \sinh \alpha_m y) \\ & + \sum_n \beta_n^{-1} \sinh \beta_n x (C_{2n} \cos \beta_n y + S_{2n} \sin \beta_n y) \quad . \end{aligned} \quad (23)$$

The expression (23) has been set up so that the C's and S's are dimensionless and $\partial\psi_x/\partial x$ [which appears in the first three equations of (14)] has essentially the standard Fourier series form in each of x and y .

b. Construction of ϕ . Let the functions ϕ' , ϕ'' , and $\bar{\phi}$ be such that [see (12)]

$$\phi = \phi' + \phi'' + \bar{\phi} \quad ; \quad (24)$$

$$\frac{\partial^2 \phi'}{\partial x^2} + \frac{\partial^2 \phi'}{\partial y^2} = 0 \quad ; \quad (25)$$

^{*}An arbitrary constant can be added to the stress functions without altering the stress or displacement fields, so k_0 can be ignored.

$$\frac{\partial^2 \phi''}{\partial x^2} + \frac{\partial^2 \phi''}{\partial y^2} = 0 \quad ; \quad (26)$$

$$\frac{\partial^2 \bar{\phi}}{\partial x^2} + \frac{\partial^2 \bar{\phi}}{\partial y^2} = \frac{1 + \nu}{1 - \nu} \alpha T \quad . \quad (27)$$

The function ϕ' will be set up following the same line of reasoning as for ψ_x ; the function $\bar{\phi}$ is to be a particular solution corresponding to the temperature distribution (8), and ϕ'' will be constructed in such a way as to eliminate terms in the equations representing the boundary conditions that do not lend themselves easily to Fourier series methods.

c. Construction of ϕ' . Following the same procedure as in a, but noting that ϕ should be an even function of x , leads us to take ϕ' in the form

$$\begin{aligned} \phi' = & C_2 ay + \frac{1}{2} C_3(x^2 - y^2) \\ & + \sum_m \alpha_m^{-2} \cos \alpha_m x (C_{3m} \cosh \alpha_m y + S_{3m} \sinh \alpha_m y) \\ & + \sum_n \beta_n^{-2} \cosh \beta_n x (C_{4n} \cos \beta_n y + S_{4n} \sin \beta_n y) \quad , \end{aligned} \quad (28)$$

which has been set up so that the C's and S's are dimensionless and $\partial^2 \phi' / \partial x^2$, and $\partial^2 \phi' / \partial y^2$, needed for σ_{xx} and σ_{yy} , respectively [see (14)], look like the sums of Fourier series in x and y . Note that $x^2 - y^2$ is a solution to (25) not obtainable using the method of separation of variables.

d. Construction of $\bar{\phi}$. Referring to (8), it is easily verified that

$$\begin{aligned} \bar{\phi} = & \frac{1}{2} A_0 x^2 - \sum_m A_{m0} \alpha_m^{-2} \cos \alpha_m x \\ & - \sum_n \beta_n^{-2} (A_{0n} \cos \beta_n y + B_{0n} \sin \beta_n y) \\ & - \sum_m \sum_n (\alpha_m^2 + \beta_n^2)^{-1} \cos \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \end{aligned} \quad (29)$$

is a particular solution to (27).

e. Construction of ϕ'' . In order to use Fourier series methods to satisfy the boundary conditions, we want the stresses as given by (14) to look like Fourier series. Inspection of (14) shows that the stresses can be considered to be functions of $\phi + x\psi_x$ and ψ_x . Now ψ_x has the proper Fourier series form, but $\phi + x\psi_x$ does not unless part of ϕ cancels out the unwanted terms arising from $x\psi_x$. The function ϕ'' will be constructed to provide the cancellation.

If $f(x,y)$ is a harmonic function, then $x \frac{\partial f}{\partial x} + y \frac{\partial f}{\partial y}$ is harmonic also. Applying this information to a function similar to (28), it follows that*

$$\begin{aligned}\phi'' = & \sum_m \alpha_m^{-1} [C_{5m} (x \sin \alpha_m x \cosh \alpha_m y - y \cos \alpha_m x \sinh \alpha_m y) \\ & + S_{5m} (x \sin \alpha_m x \sinh \alpha_m y - y \cos \alpha_m x \cosh \alpha_m y)] \\ & + \sum_n \beta_n^{-1} [C_{6n} (x \sinh \beta_n x \cos \beta_n y - y \cosh \beta_n x \sin \beta_n y) \\ & + S_{6n} (x \sinh \beta_n x \sin \beta_n y + y \cosh \beta_n x \cos \beta_n y)]\end{aligned}\quad (30)$$

is a solution to (26). From (23) and (30) we obtain

$$\begin{aligned}\phi'' + x\psi_x = & \frac{1}{2} C_1 x^2 \\ & + \sum_m \alpha_m^{-1} [(C_{5m} + C_{1m}) x \sin \alpha_m x \cosh \alpha_m y - C_{5m} y \cos \alpha_m x \sinh \alpha_m y] \\ & + \sum_m \alpha_m^{-1} [(S_{5m} + S_{1m}) x \sin \alpha_m x \sinh \alpha_m y - S_{5m} y \cos \alpha_m x \cosh \alpha_m y] \\ & + \sum_n \beta_n^{-1} [(C_{6n} + C_{2n}) x \sinh \beta_n x \cos \beta_n y - C_{6n} y \cosh \beta_n x \sin \beta_n y] \\ & + \sum_n \beta_n^{-1} [(S_{6n} + S_{2n}) x \sinh \beta_n x \sin \beta_n y + S_{6n} y \cosh \beta_n x \cos \beta_n y]\end{aligned}\quad (31)$$

The undesirable terms are those containing $x \sin \alpha_m x$, $y \sin \beta_n y$, and $y \cos \beta_n y$. They can be eliminated by taking

$$C_{5m} = -C_{1m} \quad ; \quad S_{5m} = -S_{1m} \quad ; \quad C_{6n} = S_{6n} = 0 \quad . \quad (32)$$

*Note that this solution cannot be obtained by using separation of variables

f. Final Form of $\phi + x\psi_x$. By means of (23), (24), (28), (29), (30), and (32), we arrive at

$$\begin{aligned}
 \phi + x\psi_x = & C_2ay + \frac{1}{2} (A_0 + C_1 + C_3) x^2 - \frac{1}{2} C_3 y^2 \\
 & - \sum_m A_{m0} \alpha_m^{-2} \cos \alpha_m x \\
 & - \sum_n \beta_n^{-2} (A_{0n} \cos \beta_n y + B_{0n} \sin \beta_n y) \\
 & - \sum_m \sum_n (\alpha_m^2 + \beta_n^2)^{-1} \cos \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \\
 & + \sum_m \alpha_m^{-2} \cos \alpha_m x (C_{3m} \cosh \alpha_m y + C_{1m} \alpha_m y \sinh \alpha_m y) \\
 & + \sum_m \alpha_m^{-2} \cos \alpha_m x (S_{3m} \sinh \alpha_m y + S_{1m} \alpha_m y \cosh \alpha_m y) \\
 & + \sum_n \beta_n^{-2} \cos \beta_n y (C_{4n} \cosh \beta_n x + C_{2n} \beta_n x \sinh \beta_n x) \\
 & + \sum_n \beta_n^{-2} \sin \beta_n y (S_{4n} \cosh \beta_n x + S_{2n} \beta_n x \sinh \beta_n x) \quad . \quad (33)
 \end{aligned}$$

4. Evaluation of Arbitrary Constant Using the Boundary Conditions

a. Boundary Conditions in Terms of Arbitrary Constants. The displacements and stresses found by substituting (23), (33), and (8) into (13), and (14) satisfy the field equations (1), and (2) for arbitrary C_1 , C_2 , C_3 , C_{1m} , C_{2n} , C_{3m} , C_{4n} , S_{1m} , S_{2n} , S_{3m} , and S_{4n} . The values of these constants will be determined in satisfying the requirement that the stress field meet the boundary conditions (16)-(21). To illustrate the technique used, the operations on the boundary condition (16) will be treated in detail here. Substituting (23), (33), and (8) into the first of (14), evaluating the result at $x = a$, and applying (16) results in

$$\begin{aligned}
& - (1 - \nu)C_1 + C_3 \\
& - \sum_m (-1)^m \left\{ [2(2 - \nu)C_{1m} + C_{3m}] \cosh \alpha_m y + C_{1m} \alpha_m y \sinh \alpha_m y \right\} \\
& - \sum_m (-1)^m \left\{ [2(2 - \nu)S_{1m} + S_{3m}] \sinh \alpha_m y + S_{1m} \alpha_m y \cosh \alpha_m y \right\} \\
& + \sum_n \cos \beta_n y \left\{ C_{2n} [-2(1 - \nu) \cosh \beta_n a + \beta_n a \sinh \beta_n a] + C_{4n} \cosh \beta_n a \right\} \\
& + \sum_n \sin \beta_n y \left\{ S_{2n} [-2(1 - \nu) \cosh \beta_n a + \beta_n a \sinh \beta_n a] + S_{4n} \cosh \beta_n a \right\} \\
& = P_1 + \sum_n [(A_{0n} + P_{1n}) \cos \beta_n y + (B_{0n} + Q_{1n}) \sin \beta_n y] \\
& + \sum_m \sum_n (-1)^m \beta_n^2 (\alpha_m^2 + \beta_n^2)^{-1} (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \quad . \quad (34)
\end{aligned}$$

b. Fourier Analysis. Following familiar Fourier series methods, multiply (34) by $\frac{1}{2}b^{-1}$, $b^{-1} \cos \beta_j y$, and $b^{-1} \sin \beta_j y$, respectively, and each time integrate with respect to y from $-b$ to b . This procedure yields

$$\begin{aligned}
& - (1 - \nu)C_1 + C_3 \\
& - \sum_m (-1)^m (\alpha_m b)^{-1} \left\{ C_{1m} [(3 - 2\nu) \sinh \alpha_m b + \alpha_m b \cosh \alpha_m b] \right. \\
& \quad \left. + C_{3m} \sinh \alpha_m b \right\} \\
& = P_1 \quad ; \quad (35)
\end{aligned}$$

$$\begin{aligned}
& - \sum_m 2(-1)^j (-1)^m \alpha_m (\alpha_m^2 + \beta_j^2)^{-1} b^{-1} \left[C_{1m} \left\{ [3 - 2\nu + 2\beta_j^2 (\alpha_m^2 + \beta_j^2)^{-1}] \sinh \alpha_m b \right. \right. \\
& \quad \left. \left. + \alpha_m b \cosh \alpha_m b \right\} + C_{3m} \sinh \alpha_m b \right] \\
& + C_{2j} [-2(1 - \nu) \cosh \beta_j a + \beta_j a \sinh \beta_j a] + C_{4j} \cosh \beta_j a \\
& = A_{0j} + P_{1j} + \sum_m (-1)^m \beta_j^2 (\alpha_m^2 + \beta_j^2)^{-1} A_{mj} \quad ; \quad (36)
\end{aligned}$$

$$\begin{aligned}
& \sum_m 2(-1)^j(-1)^m \beta_j (\alpha_m^2 + \beta_j^2)^{-1} b^{-1} \left[S_{1m} \left\{ [2(1-\nu) + 2\beta_j^2 (\alpha_m^2 + \beta_j^2)^{-1}] \sinh \alpha_m b \right. \right. \\
& \left. \left. + \alpha_m b \cosh \alpha_m b \right\} + S_{3m} \sinh \alpha_m b \right] \\
& S_{2j} [-2(1-\nu) \cosh \beta_j a + \beta_j a \sinh \beta_j a] + S_{4j} \cosh \beta_j a \\
& = B_{0j} + Q_{1j} + \sum_m (-1)^m \beta_j^2 (\alpha_m^2 + \beta_j^2)^{-1} B_{mj} \quad .
\end{aligned} \tag{37}$$

c. Solution for C's and S's. Equations (35), (36), (37), and those resulting from similar operations on the boundary conditions (17)-(21) are ten simultaneous equations in the ten unknowns $C_1, C_3, C_{1m}, C_{2n}, C_{3m}, C_{4n}, S_{1m}, S_{2n}, S_{3m},$ and S_{4n} . Their solution is

$$C_1 = - (A_0 + P_1 + P_2) \quad ; \tag{38}$$

$$C_3 = - (1-\nu)(A_0 + P_2) + \nu P_1 \quad ; \tag{39}$$

$$C_{2n} = - \sinh \beta_n a (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1}$$

$$\begin{aligned}
& \cdot [4(-1)^n \beta_n^2 b^{-1} \sum_m (-1)^m \alpha_m (\alpha_m^2 + \beta_n^2)^{-2} \sinh \alpha_m b C_{1m} \\
& + A_{0n} + P_{1n} + \beta_n^2 \sum_m (-1)^m (\alpha_m^2 + \beta_n^2)^{-1} A_{mn}] \quad ;
\end{aligned} \tag{40}$$

$$C_{3m} = - C_{1m} (3-2\nu + \alpha_m b \operatorname{ctnh} \alpha_m b) \quad ; \tag{41}$$

$$C_{4n} = C_{2n} (1-2\nu - \beta_n a \operatorname{ctnh} \beta_n a) \quad ; \tag{42}$$

$$S_{2n} = \sinh \beta_n a (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1}$$

$$\begin{aligned}
& \cdot \left\{ 4(-1)^n \beta_n^3 b^{-1} \sum_m (-1)^m (\alpha_m^2 + \beta_n^2)^{-2} \sinh \alpha_m b S_{1m} \right. \\
& \left. - B_{0n} - Q_{1n} - \beta_n b^{-1} \sum_m (-1)^m (\alpha_m^2 + \beta_n^2)^{-1} [\beta_n b B_{mn} + (-1)^n (P_{3m} - P_{2m})] \right\} \quad ;
\end{aligned} \tag{43}$$

$$S_{3m} = -S_{1m} [2(1-\nu) + \alpha_m b \operatorname{ctnh} \alpha_m b] + \frac{1}{2} (P_{2m} - P_{3m}) (\sinh \alpha_m b)^{-1} \quad ; \tag{44}$$

$$S_{4n} = S_{2n} (1 - 2\nu - \beta_n a \operatorname{ctnh} \beta_n a) \quad , \quad (45)$$

where C_{1i} , S_{1i} are the solutions of

$$\begin{aligned} & C_{1i} (\alpha_i b + \sinh \alpha_i b \cosh \alpha_i b) (\sinh \alpha_i b)^{-1} \\ & - 16(-1)^i \alpha_i^2 (ab)^{-1} \sum_m \sum_n (-1)^m \alpha_m \beta_n^3 (\alpha_i^2 + \beta_n^2)^{-2} (\alpha_m^2 + \beta_n^2)^{-2} \\ & \cdot \sinh^2 \beta_n a \sinh \alpha_m b (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} C_{1m} \\ & = -\frac{1}{2} (P_{2i} + P_{3i}) - A_{i0} - \alpha_i^2 \sum_n (-1)^n (\alpha_i^2 + \beta_n^2)^{-1} A_{in} \\ & + 4(-1)^i \alpha_i^2 a^{-1} \sum_n (-1)^n \beta_n (\alpha_i^2 + \beta_n^2)^{-2} \sinh^2 \beta_n a (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} (A_{0n} + P_{1n}) \\ & + 4(-1)^i \alpha_i^2 a^{-1} \sum_m \sum_n (-1)^m (-1)^n \beta_n^3 (\alpha_i^2 + \beta_n^2)^{-2} (\alpha_m^2 + \beta_n^2)^{-1} \sinh^2 \beta_n a \\ & \cdot (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} A_{mn} \quad ; \end{aligned} \quad (46)$$

$$\begin{aligned} & S_{1i} (\alpha_i b - \sinh \alpha_i b \cosh \alpha_i b) (\sinh \alpha_i b)^{-1} \\ & + 16(-1)^i \alpha_i (ab)^{-1} \sum_m \sum_n (-1)^m \beta_n^5 (\alpha_i^2 + \beta_n^2)^{-2} (\alpha_m^2 + \beta_n^2)^{-2} \sinh^2 \beta_n a \\ & \cdot \sinh \alpha_m b (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} S_{1m} \\ & = \frac{1}{2} (P_{2i} - P_{3i}) \operatorname{ctnh} \alpha_i b - \alpha_i \sum_n (-1)^n \beta_n (\alpha_i^2 + \beta_n^2)^{-1} B_{in} \\ & + 4(-1)^i \alpha_i a^{-1} \sum_n (-1)^n \beta_n^2 (\alpha_i^2 + \beta_n^2)^{-2} \sinh^2 \beta_n a (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} (B_{0n} + Q_{in}) \\ & + 4(-1)^i \alpha_i (ab)^{-1} \sum_m \sum_n (-1)^m \beta_n^3 (\alpha_i^2 + \beta_n^2)^{-2} (\alpha_m^2 + \beta_n^2)^{-1} \sinh^2 \beta_n a \\ & \cdot (\beta_n a + \sinh \beta_n a \cosh \beta_n a)^{-1} [(-1)^n \beta_n b B_{mn} + P_{3m} - P_{2m}] \quad . \end{aligned} \quad (47)$$

Note that the C 's, which correspond to the part of the solution which is an even function of y , are independent of the S 's, which correspond to the part of the solution which is an odd function of y .

d. Numerical Evaluation of C's and S's. Equation (46) represents an infinite set of linear algebraic equations in the constants* C_{1m} , $m = 1, 2, 3 \dots$. The assumption that C_{1m} is of negligible significance for $m > r$ leads to a set of r linear algebraic equations in the r unknowns $C_{11}, C_{12}, C_{13}, \dots, C_{1r}$, which can be easily solved on a digital computer for quite large values of r . Substitution of these results into (40), (41), and (42) gives the corresponding values of C_{2n} , C_{3m} , and C_{4n} . A similar procedure based on equations (47), (43), (44), and (45) gives S_{1m} , S_{2n} , S_{3m} , and S_{4n} .

5. Final Expressions for the Displacements and Stresses

Using equations (13), (14), (8), (23), (33), (38), (39), (41), (42), (44) and (45), the displacements and stresses in terms of C_{1m} , C_{2n} , S_{1m} , and S_{2n} are

$$\begin{aligned}
 u_x = & [(1 - \nu)(A_0 + P_1) - \nu P_2] x \\
 & + \sum_m \alpha_m^{-1} A_{m0} \sin \alpha_m x \\
 & + \sum_m \sum_n \alpha_m (\alpha_m^2 + \beta_n^2)^{-1} \sin \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \\
 & + \frac{1}{2} \sum_m (\alpha_m \sinh \alpha_m b)^{-1} (P_{3m} - P_{2m}) \sin \alpha_m x \sinh \alpha_m y \\
 & + \sum_m \alpha_m^{-1} C_{1m} \sin \alpha_m x \left\{ [-(1 - 2\nu) + \alpha_m b \operatorname{ctnh} \alpha_m b] \cosh \alpha_m y \right. \\
 & \quad \left. - \alpha_m y \sinh \alpha_m y \right\} \\
 & + \sum_m \alpha_m^{-1} S_{1m} \sin \alpha_m x \left\{ [-2(1 - \nu) + \alpha_m b \operatorname{ctnh} \alpha_m b] \sinh \alpha_m y \right. \\
 & \quad \left. - \alpha_m y \cosh \alpha_m y \right\} \\
 & + \sum_n \beta_n^{-1} (C_{2n} \cos \beta_n y + S_{2n} \sin \beta_n y) \cdot \\
 & \quad \left\{ -[2(1 - \nu) + \beta_n a \operatorname{ctnh} \beta_n a] \sinh \beta_n x + \beta_n x \cosh \beta_n x \right\} \quad ; \quad (48)
 \end{aligned}$$

*Remember that the A's and B's are known from the prescribed temperature distribution and the P's and Q's are known from the prescribed boundary loading.

$$\begin{aligned}
u_y = & C_2 a [(1 - \nu) (A_0 + P_2) - \nu P_1] y \\
& + \sum_n \beta_n^{-1} (A_{0n} \sin \beta_n y - B_{0n} \cos \beta_n y) \\
& + \sum_m \sum_n \beta_n (\alpha_m^2 + \beta_n^2)^{-1} \cos \alpha_m x (A_{mn} \sin \beta_n y - B_{mn} \cos \beta_n y) \\
& + \frac{1}{2} \sum_m (\alpha_m \sinh \alpha_m b)^{-1} (P_{2m} - P_{3m}) \cos \alpha_m x \cosh \alpha_m y \\
& + \sum_m \alpha_m^{-1} C_{1m} \cos \alpha_m x \left\{ -[2(1 - \nu) + \alpha_m b \operatorname{ctnh} \alpha_m b] \sinh \alpha_m y \right. \\
& \left. + \alpha_m y \cosh \alpha_m y \right\} \\
& + \sum_m \alpha_m^{-1} S_{1m} \cos \alpha_m x [-(1 - 2\nu + \alpha_m b \operatorname{ctnh} \alpha_m b) \cosh \alpha_m y \\
& + \alpha_m y \sinh \alpha_m y] \\
& + \sum_n \beta_n^{-1} (C_{2n} \sin \beta_n y - S_{2n} \cos \beta_n y) \left\{ [-(1 - 2\nu) + \beta_n a \operatorname{ctnh} \beta_n a] \right. \\
& \left. \cosh \beta_n x - \beta_n x \sinh \beta_n x \right\} \quad ; \tag{49}
\end{aligned}$$

$$\begin{aligned}
\frac{\sigma_{xx}}{2\mu} = & P_1 - \sum_n (A_{0n} \cos \beta_n y + B_{0n} \sin \beta_n y) \\
& - \sum_m \sum_n \beta_n^2 (\alpha_m^2 + \beta_n^2)^{-1} \cos \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \\
& + \frac{1}{2} \sum_m (P_{3m} - P_{2m}) (\sinh \alpha_m b)^{-1} \cos \alpha_m x \sinh \alpha_m y \\
& + \sum_m C_{1m} \cos \alpha_m x [(-1 + \alpha_m b \operatorname{ctnh} \alpha_m b) \cosh \alpha_m y - \alpha_m y \sinh \alpha_m y] \\
& + \sum_m S_{1m} \cos \alpha_m x [(-2 + \alpha_m b \operatorname{ctnh} \alpha_m b) \sinh \alpha_m y - \alpha_m y \cosh \alpha_m y] \\
& + \sum_n (C_{2n} \cos \beta_n y + S_{2n} \sin \beta_n y) [-(1 + \beta_n a \operatorname{ctnh} \beta_n a) \cosh \beta_n x \\
& + \beta_n x \sinh \beta_n x] \quad ; \tag{50}
\end{aligned}$$

$$\begin{aligned}
\frac{\sigma_{yy}}{2\mu} = & P_2 - \sum_m A_{m0} \cos \alpha_m x \\
& - \sum_m \sum_n \alpha_m^2 (\alpha_m^2 + \beta_n^2)^{-1} \cos \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \\
& + \frac{1}{2} \sum_m (P_{2m} - P_{3m}) (\sinh \alpha_m b)^{-1} \cos \alpha_m x \sinh \alpha_m y \\
& + \sum_m C_{1m} \cos \alpha_m x [-(1 + \alpha_m b \operatorname{ctnh} \alpha_m b) \cosh \alpha_m y + \alpha_m y \sinh \alpha_m y] \\
& + \sum_m S_{1m} \cos \alpha_m x (-\alpha_m b \operatorname{ctnh} \alpha_m b \sinh \alpha_m y + \alpha_m y \cosh \alpha_m y) \\
& + \sum_n (C_{2n} \cos \beta_n y + S_{2n} \sin \beta_n y) [(-1 + \beta_n a \operatorname{ctnh} \beta_n a) \cosh \beta_n x \\
& - \beta_n x \sinh \beta_n x] \quad ; \tag{51}
\end{aligned}$$

$$\begin{aligned}
\frac{\sigma_{xy}}{2\mu} = & \sum_m \sum_n \alpha_m \beta_n (\alpha_m^2 + \beta_n^2)^{-1} \sin \alpha_m x (-A_{mn} \sin \beta_n y + B_{mn} \cos \beta_n y) \\
& + \frac{1}{2} \sum_m (P_{3m} - P_{2m}) (\sinh \alpha_m b)^{-1} \sin \alpha_m x \cosh \alpha_m y \\
& + \sum_m C_{1m} \sin \alpha_m x (\alpha_m b \operatorname{ctn} \alpha_m b \sinh \alpha_m y - \alpha_m y \cosh \alpha_m y) \\
& + \sum_m S_{1m} \sin \alpha_m x [(-1 + \alpha_m b \operatorname{ctnh} \alpha_m b) \cosh \alpha_m y - \alpha_m y \sinh \alpha_m y] \\
& + \sum_n (C_{2n} \sin \beta_n y - S_{2n} \cos \beta_n y) (\beta_n a \operatorname{ctnh} \beta_n a \sinh \beta_n x \\
& - \beta_n x \cosh \beta_n x) \quad ; \tag{52}
\end{aligned}$$

$$\begin{aligned}
\frac{\sigma_{zz}}{2\mu} = & - (1 - \nu) A_0 + \nu(P_1 + P_2) - \sum_m A_{m0} \cos \alpha_m x \\
& - \sum_n (A_{0n} \cos \beta_n y + B_{0n} \sin \beta_n y) \\
& - \sum_m \sum_n \cos \alpha_m x (A_{mn} \cos \beta_n y + B_{mn} \sin \beta_n y) \\
& - 2\nu \sum_m \cos \alpha_m x (C_{1m} \cosh \alpha_m y + S_{1m} \sinh \alpha_m y) \\
& - 2\nu \sum_n \cosh \beta_n x (C_{2n} \cos \beta_n y + S_{2n} \sin \beta_n y) \quad . \quad (53)
\end{aligned}$$

Note from equation (49) that u_y is determined only to within an arbitrary rigid body displacement C_2 . The coefficients C_{1m} and S_{1m} are found from equations (46) and (47) as described above, whereas C_{2n} and S_{2n} are found from equations (40) and (43).

B. Approximations to the Plane Strain Elasticity Solution

1. Introduction

In Part A, the plane strain quasistatic stresses and displacements were found for an elastic fuel plate having a general thermal and mechanical loading. This solution was exact, within the usual assumptions of thermo-elasticity theory; in particular, no thin-plate approximations were used because it was felt that these would blur out the effects of steep temperature gradients through the thickness. Thus, the results are valid for any ratio of plate length to thickness and are not restricted to "plates." However, significant simplifications can be made in these results if it is assumed that: (a) the temperature distribution and surface loading along the length of the plate have no wild fluctuations or steep gradients; and (b) the ratio of length to thickness is large (typical fuel plate dimensions give a ratio of about 500). These simplifications will be presented here.

2. Nature of Approximation

Three schemes seemed promising for approximating the exact solution of the problem. They were:

a. Expansion of the solution in powers of the ratio of plate thickness to length and obtaining an approximation which would satisfy the differential equations (1), and (2), and the boundary conditions (16)-(21) to

within a certain power of this ratio. This did not prove feasible, as the accuracy of the approximation varied significantly along the length of the plate; moreover, the power series became nonconvergent as the ends of plate were approached.

b. Finding an approximation which would meet the boundary conditions exactly but the differential equations only approximately. This can be done, but seems unwise. First, it is difficult to estimate the accuracy to which the differential equations are satisfied, since this is a complicated function of position. In addition, it is not clear what this type of approximation means physically. Thirdly, the results might be erroneously applied in cases where the plate proportions would not justify their use - the satisfaction of the boundary conditions would make a plot of the derived stress field look quite reasonable, while the lack of satisfaction of the governing differential equations would remain hidden beneath the surface.

c. Finding an approximation which would satisfy the differential equations exactly, but the boundary conditions only approximately. Although involving much the same mathematical effort as b, this approach would seem to give more useful results. The nature of the approximation is physically clear, and any misuse of the results would be quickly revealed by a plot of the stress field obtained. This is therefore the approximation scheme that will be used here.

From the exact solution we know that the displacements and stresses given by equations (48)-(53) satisfy the differential equations (1), and (2) for any choice of the constants C_{1m} , C_{2n} , S_{1m} , and S_{2n} . These constants were then determined so as to satisfy the boundary conditions (16)-(21) exactly, the result being infinite sets of simultaneous algebraic equations, (46), and (47), for C_{1m} and S_{1m} . We will now find approximate solutions to these sets of equations in the hope of obtaining values for C_{1m} , C_{2n} , S_{1m} , and S_{2n} that yield stresses on the boundary that are good approximations to the prescribed boundary conditions.

Define R , α_{mn} , $\bar{C}_{1m}$, $\bar{C}_{2n}$, $\bar{S}_{1m}$, and $\bar{S}_{2n}$ by

$$\begin{aligned}
 R &= b/a \quad ; \quad \alpha_{mn} = \left[1 + \left(\frac{n}{mR} \right)^2 \right]^{-1} \quad ; \quad \bar{C}_{1m} = C_{1m} \frac{\sinh \alpha_m b}{G(\alpha_m b)} \quad ; \\
 \bar{C}_{2n} &= C_{2n} \frac{\sinh \beta_n a}{G(\beta_n a)} \quad ; \quad \bar{S}_{1m} = S_{1m} \frac{\sinh \alpha_m b}{H(\alpha_m b)} \quad ; \quad \text{and} \\
 \bar{S}_{2n} &= S_{2n} \frac{\sinh \beta_n a}{G(\beta_n a)} \quad , \quad (54)
 \end{aligned}$$

where

$$G(X) = \frac{\sinh^2 X}{\sinh X \cosh X + X} \quad ; \quad H(X) = \frac{\sinh^2 X}{\sinh X \cosh X - X} \quad .$$

It will be recalled that b is half the plate length and a is half the plate thickness, so that R is a large number. Using this notation and equation (9), we obtain for equations (46), (40), (47), and (43),

$$\begin{aligned} \bar{C}_{1m} = & -\frac{1}{2} (P_{2m} + P_{3m}) - A_{m0} - \sum_n (-1)^n \alpha_{mn} A_{mn} \\ & + \sum_n 4(-1)^m (-1)^n n \alpha_{mn}^2 (m^2 \pi R)^{-1} G\left(\frac{n\pi}{R}\right) [A_{0n} + P_{1n}] \\ & + \sum_i \sum_n 4(-1)^i (-1)^m (-1)^n n^3 \alpha_{mn}^2 \alpha_{in} (m^2 i^2 \pi R^3)^{-1} G\left(\frac{n\pi}{R}\right) A_{in} \\ & + \sum_i \sum_n 16(-1)^i (-1)^m n^3 \alpha_{mn}^2 \alpha_{in}^2 (m^2 i^3 \pi^2 R^4)^{-1} G\left(\frac{n\pi}{R}\right) G(i\pi R) \bar{C}_{1i} \quad ; \\ \bar{C}_{2n} = & - (A_{0n} + P_{1n}) - \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} A_{mn} \\ & - \sum_m 4(-1)^m (-1)^n n^2 \alpha_{mn}^2 (m^3 \pi R^3)^{-1} G(m\pi R) \bar{C}_{1m} \quad ; \\ \bar{S}_{1m} = & \frac{1}{2} (P_{3m} - P_{2m}) \operatorname{ctnh} m\pi R + \sum_n (-1)^n n \alpha_{mn} (mR)^{-1} B_{mn} \\ & - \sum_n 4(-1)^m (-1)^n n^2 \alpha_{mn}^2 (m^3 \pi R^2)^{-1} G\left(\frac{n\pi}{R}\right) [B_{0n} + Q_{1n}] \\ & - \sum_i \sum_n 4(-1)^i (-1)^m n^3 \alpha_{mn}^2 \alpha_{in} (m^3 i^2 \pi^2 R^4)^{-1} G\left(\frac{n\pi}{R}\right) [(-1)^n n \pi B_{in} + P_{3i} - P_{2i}] \\ & + \sum_i \sum_n 16(-1)^i (-1)^m n^5 \alpha_{mn}^2 \alpha_{in}^2 (m^3 i^4 \pi^2 R^6)^{-1} G\left(\frac{n\pi}{R}\right) H(i\pi R) \bar{S}_{1i} \quad ; \\ \bar{S}_{2n} = & - (B_{0n} + Q_{1n}) - \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} B_{mn} \\ & + \sum_m (-1)^m (-1)^n n \alpha_{mn} (m^2 \pi R^2)^{-1} (P_{2m} - P_{3m}) \\ & + \sum_m 4(-1)^m (-1)^n n^3 \alpha_{mn}^2 (m^4 \pi R^4)^{-1} H(m\pi R) \bar{S}_{1m} \end{aligned} \quad (55)$$

In the expressions (48)-(53) for the displacements and stresses, the functions

$$\frac{\cosh \alpha_m y}{\sinh \alpha_m b} = \frac{\cosh \frac{m \pi R y}{b}}{\sinh m \pi R} = \frac{\exp [-m \pi R (1 - \frac{|y|}{b})] + \exp [-m \pi R (1 + \frac{|y|}{b})]}{1 - \exp (-2m \pi R)} ;$$

$$\frac{\sinh \alpha_m y}{\sinh \alpha_m b} = \frac{\sinh \frac{m \pi R y}{b}}{\sinh m \pi R} = \frac{y}{|y|} \frac{\exp [-m \pi R (1 - \frac{|y|}{b})] - \exp [-m \pi R (1 + \frac{|y|}{b})]}{1 - \exp (-2m \pi R)} ;$$
(56)

$m = 1, 2, 3 \dots$

occur frequently. Here $y/|y|$ is just a device to indicate the sign of y and is defined by

$$\frac{y}{|y|} = 1 \quad , \quad y \geq 0$$

$$= -1 \quad , \quad y < 0 \quad .$$
(57)

Since R is very large, considerable simplification can be made in (56). Even if mR were as small as 5, say, $\exp (-2 m \pi R)$ would be roughly 10^{-14} and hence negligible compared with 1. Similarly, $\exp [-m \pi R (1 + \frac{|y|}{b})]$ would vary between 10^{-7} and 10^{-14} as $|y|$ varied between 0 and b , and so will also be neglected. On the other hand, $\exp [-m \pi R (1 - \frac{|y|}{b})]$ has the value 1 at $|y| = b$ and will be retained. Thus, we will make the approximations

$$\cosh \alpha_m y / \sinh \alpha_m b \approx e^{-m f} \quad ;$$

$$\sinh \alpha_m y / \sinh \alpha_m b \approx (y/|y|) e^{-m f} \quad ;$$

$$G(\alpha_m b) \approx H(\alpha_m b) \approx \operatorname{ctnh} \alpha_m b \approx 1 \quad ,$$
(58)

where

$$f(y) = \pi R (1 - \frac{|y|}{b}) \quad .$$
(59)

The substitution of (54), and (58) into (48)-(53) yields

$$\begin{aligned}
 \frac{u_x}{a} &= [(1 - \nu)(A_0 + P_1) - \nu P_2] \frac{x}{a} \\
 &+ \sum_m \sum_n (m\pi)^{-1} \alpha_{mn} \sin \frac{m\pi x}{a} \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \\
 &+ \sum_m (m\pi)^{-1} \sin \frac{m\pi x}{a} \left[A_{m0} + \bar{C}_{1m} [-(1 - 2\nu) + mf] e^{-mf} \right. \\
 &\left. + \left\{ \frac{1}{2} (P_{3m} - P_{2m}) + \bar{S}_{1m} [-2(1 - \nu) + mf] \right\} \frac{y}{|y|} e^{-mf} \right] \\
 &- \sum_n \left[\bar{C}_{2n} \cos \frac{n\pi y}{b} + \bar{S}_{2n} \sin \frac{n\pi y}{b} \right] F_1(n, x) \quad ; \\
 \\
 \frac{u_y}{b} &= \frac{C_2}{R} + [(1 - \nu)(A_0 + P_2) - \nu P_1] \frac{y}{b} \\
 &+ \sum_m \sum_n n \alpha_{mn} (m^2 \pi R^2)^{-1} \cos \frac{m\pi x}{a} \left[A_{mn} \sin \frac{n\pi y}{b} - B_{mn} \cos \frac{n\pi y}{b} \right] \\
 &+ \sum_m (m\pi R)^{-1} \cos \frac{m\pi x}{a} \left\{ -\bar{C}_{1m} [2(1 - \nu) + mf] \frac{y}{|y|} \right. \\
 &\left. + \frac{1}{2} (P_{2m} - P_{3m}) - \bar{S}_{1m} (1 - 2\nu + mf) \right\} e^{-mf} \\
 &+ \sum_n (n\pi)^{-1} \left\{ [A_{0n} + \bar{C}_{2n} F_2(n, x)] \sin \frac{n\pi y}{b} \right. \\
 &\left. - [B_{0n} + \bar{S}_{2n} F_2(n, x)] \cos \frac{n\pi y}{b} \right\} \quad ; \\
 \\
 \frac{\sigma_{xx}}{2\mu} &= P_1 - \sum_m \sum_n n^2 \alpha_{mn} (m^2 R^2)^{-1} \cos \frac{m\pi x}{a} \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \\
 &+ \sum_m \cos \frac{m\pi x}{a} \left\{ -\bar{C}_{1m} (1 - mf) + \left[\frac{1}{2} (P_{3m} - P_{2m}) - \bar{S}_{1m} (2 - mf) \right] \frac{y}{|y|} e^{-mf} \right. \\
 &\left. - \sum_n \left\{ [A_{0n} + \bar{C}_{2n} F_3(n, x)] \cos \frac{n\pi y}{b} + [B_{0n} + \bar{S}_{2n} F_3(n, x)] \sin \frac{n\pi y}{b} \right\} \right\} \quad ;
 \end{aligned}$$

$$\begin{aligned}
\frac{\sigma_{yy}}{2\mu} &= P_2 - \sum_m \sum_n \alpha_{mn} \cos \frac{m\pi x}{a} \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \\
&+ \sum_m \cos \frac{m\pi x}{a} \left\{ -A_{m0} - \bar{C}_{1m} (1 + mf) e^{-mf} \right. \\
&+ \left. \left[\frac{1}{2} (P_{2m} - P_{3m}) - \bar{S}_{1m} mf \right] \frac{y}{|y|} e^{-mf} \right\} \\
&- \sum_n \left[\bar{C}_{2n} \cos \frac{n\pi y}{b} + \bar{S}_{2n} \sin \frac{n\pi y}{b} \right] F_4(n, x) \quad ; \\
\frac{\sigma_{xy}}{2\mu} &= \sum_m \sum_n n \alpha_{mn} (mR)^{-1} \sin \frac{m\pi x}{a} \left[-A_{mn} \sin \frac{n\pi y}{b} + B_{mn} \cos \frac{n\pi y}{b} \right] \\
&+ \sum_m \sin \frac{m\pi x}{a} \left[\bar{C}_{1m} mf \frac{y}{|y|} + \frac{1}{2} (P_{3m} - P_{2m}) - \bar{S}_{1m} (1 - mf) \right] e^{-mf} \\
&+ \sum_n \left[\bar{C}_{2n} \sin \frac{n\pi y}{b} - \bar{S}_{2n} \cos \frac{n\pi y}{b} \right] F_5(n, x) \quad ;
\end{aligned}$$

and

$$\begin{aligned}
\frac{\sigma_{zz}}{2\mu} &= - (1 - \nu) A_0 + \nu (P_1 + P_2) - \sum_m \sum_n \cos \frac{m\pi x}{a} \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \\
&- \sum_m \cos \frac{m\pi x}{a} \left[A_{m0} + 2\nu \left(\bar{C}_{1m} + \bar{S}_{1m} \frac{y}{|y|} \right) e^{-mf} \right] \\
&- \sum_n \left\{ [A_{0n} + 2\nu \bar{C}_{2n} F_6(n, x)] \cos \frac{n\pi y}{b} \right. \\
&+ \left. [B_{0n} + 2\nu \bar{S}_{2n} F_6(n, x)] \sin \frac{n\pi y}{b} \right\} \quad (60)
\end{aligned}$$

The functions F_1 through F_6 are defined as

$$F_1(n, x) = \frac{\left[2(1 - \nu) \sinh \frac{n\pi}{R} + \frac{n\pi}{R} \cosh \frac{n\pi}{R} \right] \sinh \frac{n\pi x}{Ra} \sinh \frac{n\pi}{R} \cosh \frac{n\pi x}{Ra}}{\frac{n\pi}{R} \left(\sinh \frac{n\pi}{R} \cosh \frac{n\pi}{R} + \frac{n\pi}{R} \right)} \quad ;$$

$$F_2(n, x) = -(1 - 2\nu) F_6(n, x) + F_0(n, x) \quad ;$$

$$F_3(n, x) = F_6(n, x) + F_0(n, x) \quad ;$$

$$F_4(n, x) = F_6(n, x) - F_0(n, x) \quad ;$$

$$F_5(n, x) = \frac{\frac{n\pi}{R} \cosh \frac{n\pi}{R} \sinh \frac{n\pi x}{Ra} - \frac{n\pi x}{Ra} \sinh \frac{n\pi}{R} \cosh \frac{n\pi x}{Ra}}{\sinh \frac{n\pi}{R} \cosh \frac{n\pi}{R} + \frac{n\pi}{R}} ;$$

and

$$F_6(n, x) = \frac{\sinh \frac{n\pi}{R} \cosh \frac{n\pi x}{Ra}}{\sinh \frac{n\pi}{R} \cosh \frac{n\pi}{R} + \frac{n\pi}{R}} ,$$

where

$$F_0(n, x) = \frac{\frac{n\pi}{R} \cosh \frac{n\pi}{R} \cosh \frac{n\pi x}{Ra} - \frac{n\pi x}{Ra} \sinh \frac{n\pi}{R} \sinh \frac{n\pi x}{Ra}}{\sinh \frac{n\pi}{R} \cosh \frac{n\pi}{R} + \frac{n\pi}{R}} . \quad (61)$$

3. First Approximation

The exact values of $\bar{C}_{1m}$, $\bar{C}_{2n}$, $\bar{S}_{1n}$, and $\bar{S}_{2n}$ given by (55) are unwieldy to work with because of the necessity of solving the infinite sets of algebraic equations implied in the first and third of (55) and the need to evaluate the repeated summations involved therein. As a trial approximation, we will neglect the terms in (55) containing the highest powers of $1/R$, particularly as these terms contain the multiple summations. Whether this will be a good approximation depends on how well the derived stresses meet the boundary conditions (16)-(21). Denoting this first approximation to $\bar{C}_{1m}$ by $\bar{C}_{1m}^*$, etc., let us take

$$\bar{C}_{1m}^* = -\frac{1}{2} (P_{2m} + P_{3m}) - A_{m0} - \sum_n (-1)^n \alpha_{mn} A_{mn} ;$$

$$\bar{C}_{2n}^* = - (A_{0n} + P_{1n}) - \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} A_{mn} ;$$

$$\bar{S}_{1m}^* = \frac{1}{2} (P_{3m} - P_{2m}) + \sum_n (-1)^n n \alpha_{mn} (mR)^{-1} B_{mn} ;$$

and

$$\bar{S}_{2n}^* = - (B_{0n} + Q_{1n}) - \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} B_{mn} . \quad (62)$$

The substitution of (62) into (60) yields the first approximation to the displacement and stress fields, which will be denoted by u_x^* , u_y^* , σ_{xx}^* , etc. The error in the meeting of the boundary condition given by (16) is

$$\begin{aligned} & \frac{1}{2\mu} [\sigma_{xx}^* (\pm a, y) - \sigma_{xx} (\pm a, y)] \\ &= \sum_m (-1)^m \left[A_{m0} + \frac{1}{2} P_{2m} \left(1 + \frac{y}{|y|} \right) + \frac{1}{2} P_{3m} \left(1 - \frac{y}{|y|} \right) (1 - mf) \right] e^{-mf} \\ &+ \sum_m \sum_n (-1)^m (-1)^n \alpha_{mn} \left[A_{mn} (1 - mf) - B_{mn} \frac{n}{mR} (2 - mf) \frac{y}{|y|} \right] e^{-mf} . \end{aligned} \quad (63)$$

Similarly, we have for the errors in meeting the boundary conditions given by (17)-(21) the following quantities

$$\sigma_{xy}^* (\pm a, y) - \sigma_{xy} (\pm a, y) = 0 \quad ; \quad (64)$$

$$\begin{aligned} & \frac{1}{2\mu} [\sigma_{yy}^* (x, \pm b) - \sigma_{yy} (x, \pm b)] \\ &= \sum_n (-1)^n \left[A_{0n} + P_{1n} + \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} A_{mn} \right] F_4(n, x) \quad ; \end{aligned} \quad (65)$$

and

$$\begin{aligned} & \frac{1}{2\mu} [\sigma_{xy}^* (x, \pm b) - \sigma_{xy} (x, \pm b)] \\ &= \sum_n (-1)^n \left[B_{0n} + Q_{1n} + \sum_m (-1)^m n^2 \alpha_{mn} (m^2 R^2)^{-1} B_{mn} \right] F_5(n, x) . \end{aligned} \quad (66)$$

As an indication of the size of the error given by (63), Fig. VII-1 is a plot of e^{-mf} vs $|y|/b$ for various values of mR . We see that for

$R = 500$, which is typical of fuel plate proportions, e^{-mf} is negligible unless within a fraction of a percent of the length of the plate from the ends. Even for considerably smaller R (say 50), the boundary condition on σ_{xx} is met up to a very short distance from the ends of the plates.

Fig. VII-1

e^{-mf} vs $|y|/b$ for
Various Values of mR

Before looking at the errors given by (65), and (66), we must examine the implications of assumption (a) of the Introduction. If, along the length of the plate, there are no violent fluctuations in the temperature distribution and surface loadings, the Fourier series in (16) and those in (8) involving y are strongly convergent and can be truncated with good accuracy after a certain number of terms. In other words, we can take

$$A_{0n} = B_{0n} = A_{mn} = B_{mn} = P_{1n} = Q_{1n} = 0 \quad \text{for } n > N, \quad (67)$$

and the summations over n of the above quantities will be from 1 to N instead of from 1 to ∞ . Then, if $R \gg N$, we can expand $F_1(n, x)$ through $F_6(n, x)$, α_{mn} , and $G(n\pi/R)$ in powers of n/R and retain only the first few terms. This yields

$$\begin{aligned} F_1(n, x) &= \frac{x}{a} \left\{ 1 - \nu + \left(\frac{n\pi}{R} \right)^2 \nu \left(\frac{1}{6} - \frac{x^2}{a^2} \right) \right. \\ &\quad \left. + \left(\frac{n\pi}{R} \right)^4 \left[-\frac{15+\nu}{360} + \frac{3-2\nu}{3} \frac{x^2}{a^2} - (1+\nu) \frac{x^4}{a^4} \right] + \dots \right\} ; \\ F_2(n, x) &= \nu + \left(\frac{n\pi}{R} \right)^2 (1-\nu) \left(\frac{1}{6} - \frac{x^2}{2a^2} \right) \\ &\quad + \left(\frac{n\pi}{R} \right)^4 \left[-\frac{(14+\nu)}{360} + \frac{2-\nu}{12} \frac{x^2}{a^2} - \frac{2-\nu}{24} \frac{x^4}{a^4} \right] + \dots ; \\ F_3(n, x) &= 1 - \frac{1}{24} \left(\frac{n\pi}{R} \right)^4 \left(1 - \frac{x^2}{a^2} \right)^2 + \dots ; \\ F_4(n, x) &= \left(\frac{n\pi}{R} \right)^2 \left(-\frac{1}{6} + \frac{x^2}{2a^2} \right) + \left(\frac{n\pi}{R} \right)^4 \left(\frac{7}{180} - \frac{x^2}{6a^2} + \frac{x^4}{12a^4} \right) + \dots ; \\ F_5(n, x) &= \frac{x}{a} \left(1 - \frac{x^2}{a^2} \right) \left\{ \frac{1}{6} \left(\frac{n\pi}{R} \right)^3 + \frac{1}{60} \left(\frac{n\pi}{R} \right)^5 \left(-\frac{7}{3} + \frac{x^2}{a^2} \right) + \dots \right\} ; \\ F_6(n, x) &= 1 + \left(\frac{n\pi}{R} \right)^2 \left(-\frac{1}{6} + \frac{x^2}{2a^2} \right) + \left(\frac{n\pi}{R} \right)^4 \left(-\frac{1}{360} - \frac{x^2}{12a^2} + \frac{x^4}{12a^4} \right) + \dots ; \\ \alpha_{mn} &= 1 - \left(\frac{n}{mR} \right)^2 + \left(\frac{n}{mR} \right)^4 + \dots ; \\ \alpha_{mn}^2 &= 1 - 2 \left(\frac{n}{mR} \right)^2 + 3 \left(\frac{n}{mR} \right)^4 + \dots ; \end{aligned}$$

and

$$G\left(\frac{n\pi}{R}\right) = \frac{n\pi}{R} \left[1 - \frac{1}{45} \left(\frac{n\pi}{R} \right)^4 + \dots \right] \quad (68)$$

for $R \gg N \geq n$.

We can now see from (68) that the errors given by (65), and (66) are roughly of the order of R^{-2} and R^{-3} , respectively.

4. Second Approximation

If the stresses and displacements in the regions close to the ends of the plate are not of particular interest, the first approximation can be simplified by dropping all terms in $\exp(-mf)$. Figure VII-1 gives an indication of how far it is necessary to be from the ends for this to be a reasonable simplification. In addition, we will drop all terms in power of $1/R$ greater than the third. By means of (67), and (68), and the first approximation, we have for the second approximation

$$\begin{aligned} \frac{u_x^{**}}{a} = & [(1 - \nu)(A_0 + P_1) - \nu P_2] \frac{x}{a} \\ & + \sum_m \frac{A_{m0}}{m\pi} \sin \frac{m\pi x}{a} \\ & + \frac{x}{a} \sum_n^N \left[(A_{0n} + P_{1n}) \cos \frac{n\pi y}{b} + (B_{0n} + Q_{1n}) \sin \frac{n\pi y}{b} \right] \\ & \left[(1 - \nu) + \nu \left(\frac{n\pi}{R} \right)^2 \left(\frac{1}{6} - \frac{x^2}{a^2} \right) \right] \\ & + \sum_m \sum_n^N \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \\ & \left\{ \frac{1}{m\pi} \left[1 - \left(\frac{n}{mR} \right)^2 \right] \sin \frac{m\pi x}{a} + (-1)^m (1 - \nu) \frac{x}{a} \left(\frac{n}{mR} \right)^2 \right\} \quad ; (69) \end{aligned}$$

$$\begin{aligned} \frac{u_y^{**}}{b} = & \frac{C_2}{R} + [(1 - \nu)(A_0 + P_2) - \nu P_1] \frac{y}{b} \\ & + \sum_n^N \frac{1}{n\pi} \left[-P_{1n} \sin \frac{n\pi y}{b} + Q_{1n} \cos \frac{n\pi y}{b} \right] \left[\nu + (1 - \nu) \left(\frac{n\pi}{R} \right)^2 \left(\frac{1}{6} - \frac{x^2}{2a^2} \right) \right] \\ & + (1 - \nu) \sum_n^N \frac{1}{n\pi} \left[A_{0n} \sin \frac{n\pi y}{b} - B_{0n} \cos \frac{n\pi y}{b} \right] \left[1 + \left(\frac{n\pi}{R} \right)^2 \left(\frac{x^2}{2a^2} - \frac{1}{6} \right) \right] \\ & + \sum_m \sum_n^N \frac{n}{m^2 \pi R^2} \left[A_{mn} \sin \frac{n\pi y}{b} - B_{mn} \cos \frac{n\pi y}{b} \right] \left[\cos \frac{m\pi x}{a} - (-1)^m \nu \right] \quad ; \\ & (70) \end{aligned}$$

$$\begin{aligned} \frac{\sigma_{xx}^{**}}{2\mu} = & P_1 + \sum_n^N \left[P_{1n} \cos \frac{n\pi y}{b} + Q_{1n} \sin \frac{n\pi y}{b} \right] \\ & + \sum_m^N \sum_n^N \left(\frac{n}{mR} \right)^2 \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \left[(-1)^m - \cos \frac{m\pi x}{a} \right] ; \end{aligned} \quad (71)$$

$$\begin{aligned} \frac{\sigma_{yy}^{**}}{2\mu} = & P_2 - \sum_m^N A_{m0} \cos \frac{m\pi x}{a} \\ & + \sum_n^N \left(\frac{n\pi}{R} \right)^2 \left[(A_{0n} + P_{1n}) \cos \frac{n\pi y}{b} + (B_{0n} + Q_{1n}) \sin \frac{n\pi y}{b} \right] \left(-\frac{1}{6} + \frac{x^2}{2a^2} \right) \\ & - \sum_m^N \sum_n^N \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \left[1 - \left(\frac{n}{mR} \right)^2 \right] \cos \frac{m\pi x}{a} ; \end{aligned} \quad (72)$$

$$\begin{aligned} \frac{\sigma_{xy}^{**}}{2\mu} = & \frac{x}{6a} \left(1 - \frac{x^2}{a^2} \right) \sum_n^N \left(\frac{n\pi}{R} \right)^3 \left[- (A_{0n} + P_{1n}) \sin \frac{n\pi y}{b} + (B_{0n} + Q_{1n}) \cos \frac{n\pi y}{b} \right] \\ & + \sum_m^N \sum_n^N \left[- A_{mn} \sin \frac{n\pi y}{b} + B_{mn} \cos \frac{n\pi y}{b} \right] \left[\frac{n}{mR} - \left(\frac{n}{mR} \right)^3 \right] \sin \frac{m\pi x}{a} ; \end{aligned} \quad (73)$$

and

$$\begin{aligned} \frac{\sigma_{zz}^{**}}{2\mu} = & - (1 - \nu) A_0 + (P_1 + P_2) - \sum_m^N A_{m0} \cos \frac{m\pi x}{a} \\ & + \nu \sum_n^N \left[P_{1n} \cos \frac{n\pi y}{b} + Q_{1n} \sin \frac{n\pi y}{b} \right] \left[1 + \left(\frac{n\pi}{R} \right)^2 \left(-\frac{1}{6} + \frac{x^2}{2a^2} \right) \right] \\ & + \sum_n^N \left[A_{0n} \cos \frac{n\pi y}{b} + B_{0n} \sin \frac{n\pi y}{b} \right] \left[- (1 - \nu) + \nu \left(\frac{n\pi}{R} \right)^2 \left(-\frac{1}{6} + \frac{x^2}{2a^2} \right) \right] \\ & + \sum_m^N \sum_n^N \left[A_{mn} \cos \frac{n\pi y}{b} + B_{mn} \sin \frac{n\pi y}{b} \right] \left[- \cos \frac{m\pi x}{a} + \nu (-1)^m \left(\frac{n}{mR} \right)^2 \right] . \end{aligned} \quad (74)$$

We see that P_{2m} and P_{3m} , which are the coefficients of self-equilibrated loadings on the ends, do not appear in (69)-(74). This is an illustration of Saint-Venant's principle.

Note that the first approximation satisfies the governing differential equations exactly and comes "close" to meeting the boundary conditions, as discussed previously. On the other hand, the second approximation does not satisfy the differential equations nor does it even come

close to meeting the boundary conditions at the ends of the plate. It is, instead, a simplification of the first approximation, accurate away from the plate ends.

5. Effect of Lengthwise Loading Variation on Stresses

Consider the two thermal and mechanical loadings characterized by

$$\begin{aligned}
 1. \quad & A_0 = A'_0; \quad A_{m0} = A'_{m0}; \quad A_{0n} = A'_{0n}; \quad B_{0n} = B'_{0n}; \\
 & A_{mn} = A'_{mn}; \quad B_{mn} = B'_{mn}; \quad P_1 = P'_1; \quad P_{1n} = P'_{1n}; \\
 & Q_{1n} = Q'_{1n}; \quad P_2 = P'_2; \quad P_{2m} = P'_{2m}; \quad P_{3m} = P'_{3m}; \quad (75)
 \end{aligned}$$

$$2. \quad A_0 = A'_0 + \sum_n^N (A'_{0n} \cos \beta_n Y + B'_{0n} \sin \beta_n Y) \quad ;$$

$$A_{m0} = A'_{m0} + \sum_n^N (A'_{mn} \cos \beta_n Y + B'_{mn} \sin \beta_n Y) \quad ;$$

$$A_{0n} = B_{0n} = A_{mn} = B_{mn} = 0 \quad ;$$

$$P_1 = P'_1 + \sum_n^N (P'_{1n} \cos \beta_n Y + Q'_{1n} \sin \beta_n Y) \quad ;$$

$$P_2 = P'_2; \quad P_{2m} = P'_{2m}; \quad P_{3m} = P'_{3m}; \quad P_{1n} = Q_{1n} = 0 \quad . \quad (76)$$

Here Y is a constant less than b in absolute value. By (76) we see that loading 1 is a general loading in that the surface tractions and temperature distribution given by (16)-(21) and (8) are functions of both x and y . On the other hand, loading 2 gives surface traction and a temperature distribution that are independent of y . At the cross section $y = Y$, the temperature distributions and applied boundary loads of 1 and 2 are identical, but in general coincide for no other value of y . In other words, the thermal and mechanical loadings at $y = Y$ of loading 1 are applied over the whole length of the plate to obtain loading 2.

Let us assume that the second approximation, given by (69)-(74), applies and $y = Y$ is within the region of applicability. Stresses and displacement corresponding to loading 1 will be indicated by σ'_{xx} , u'_x , etc., and those corresponding to loading 2 by σ''_{xx} , u''_x , etc. Using (69)-(74) and evaluating σ'_{xx} , u'_x , etc. at $y = Y$, we find that

$$\sigma'_{xx}(x, Y) - \sigma''_{xx}(x) = O(R^{-2}) \quad ;$$

$$\sigma'_{yy}(x, Y) - \sigma''_{yy}(x) = O(R^{-2}) \quad ;$$

$$\sigma'_{zz}(x, Y) - \sigma''_{zz}(x) = O(R^{-2}) \quad ;$$

$$\sigma'_{xy}(x, Y) - \sigma''_{xy}(x) = 2\mu \sum_m \sum_n^N \left(\frac{n}{mR} \right) \left[-A_{mn} \sin \frac{n\pi Y}{b} + B_{mn} \cos \frac{n\pi Y}{b} \right] \\ + O(R^{-3}) \quad ;$$

$$u'_x(x, Y) - u''_x(x) = O(R^{-2}) \quad . \quad (77)$$

It appears, therefore, that if R is large and if we are interested in the stresses and u_x at a particular cross section $y = Y$ away from the ends of the plate, we can neglect the y variation of the temperature distribution and surface loading distribution and only need make use of the particular distributions at $y = Y$. The largest error will be in the shearing stress σ_{xy} , which comes out zero if y variations are neglected.

VIII. THERMAL STRESSES IN REACTOR FUEL PLATES

II. Thermo-elastic Stresses in a Thin, Unconstrained Plate with Time-dependent, Uniform Internal Heat Generation, Subjected to a Sudden Change in Environmental Temperature

G. Rosenberg

A. Introduction

This is the usual problem considered for the case of quenching operations, except that, during quenching, internal heat generation does not occur. The problem is of interest in considering gas-cooled reactor core elements during a startup in which significant power generation and temperature rise is realized before coolant flow begins.

In general, similar problems have been solved for the cases of steady state with internal heat generation, transient state with controlled metal boundary surface temperature and with surface heat losses through a conducting boundary. In the following treatment we consider the transient state with a uniformly distributed time dependent heat source within the plate boundaries.

B. Statement of Problem and Solution

A flat plate, containing a uniformly distributed, time-dependent heat source, having attained some uniform temperature T_0 , is suddenly exposed to a changed ambient temperature. The plate is unconstrained, infinitely long and thin. The objective is to estimate the thermo-elastic stresses as a function of time for the case where the heat is transmitted through a boundary conductance. The limiting condition (more frequently considered) for this case would be that of the sudden change in the plate surface temperature, which may provide an acceptable upper bound on the attainable thermal stress. This, however, imposes a large penalty for any approximately realistic case.

The transient state considered here is really a quasistatic state, since the temperature rise times are assumed to be much greater than any vibrational mode periods either for stress waves or plate deflections. The result is a solution for the case of a time-dependent heat source (uniformly distributed) comparable to that treated in Boley and Weiner⁴¹ without internal heat generation.

⁴¹Boley, B. A., and J. H. Weiner, Theory of Thermal Stresses, John Wiley and Sons, Inc., New York (1960), p. 284.

For the ordinary run of physically realizable situations it is a reasonable approximation to neglect the temperature change in the plate in the direction of coolant flow^{42,43*} as far as its influence on thermal stress is concerned. This assumption is used here too, although the questions associated with its use for the case of suddenly imposed coolant flow have not yet been completely resolved. For the condition of small plate width compared with core size, it is also considered acceptable to assume a uniform temperature across the plate width. This leaves the one-dimensional statement of the problem contained in the following equations:

$$\kappa \frac{\partial^2 T}{\partial x^2} + \frac{Q}{\rho c} = \frac{\partial T}{\partial t} \quad , \quad t > 0 \quad ; \quad (1)$$

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0 \quad , \quad t > 0 \quad ; \quad (2)$$

$$\left[\kappa \frac{\partial T}{\partial x} + hT \right]_{x=L} = h\bar{T} \quad , \quad t > 0 \quad ; \quad (3)$$

and

$$T = F(x) \quad , \quad \dot{t} = 0 \quad , \quad (4)$$

where

x = direction of plate thickness (measured from midplane)

L = half-plate thickness

k = conductivity

$T = T(x,t)$, temperature

Q = heat source function, $Q(t)$

h = surface heat transfer coefficient

κ = thermal diffusivity ($k/\rho c$)

t = time

ρ = density

⁴²Boley, B. A., The Determination of Temperature, Stresses and Deflections in Two-dimensional Problems, J. Aero. Sci., 67-75 (Jan 1956)

⁴³Reactor Handbook, Engineering, AECD-3646, Vol. 2 (May 1955).

*See preceding treatment: Sect. VII, Thermal Stresses in Reactor Fuel Plates: I. The Plane Strain Elasticity Solution, C. K. Youngdahl.

c = specific heat

$\bar{T}$ = ambient temperature (uniform)

$T_0 = T(x, 0)$, initial plate temperature

$\Delta T = T - \bar{T}$.

With some computational complications, the physical properties of the plate, the heat source function, and the ambient temperature may be found as functions of position. However, we only consider constant properties for this analysis, as well as a constant Q with respect to position, which is justified by the "thin plate" assumption.

Letting $\Delta T(x, t) = T(x, t) - \bar{T}$, with $\bar{T}$ a constant, equations (1) through (4) are replaced by

$$\kappa \frac{\partial^2 T(x, t)}{\partial x^2} + \frac{Q(t)}{\rho c} = \frac{\partial \Delta T(x, t)}{\partial t}, \quad t > 0; \quad (1a)$$

$$\left[\frac{\partial \Delta T(x, t)}{\partial x} \right]_{x=0} = 0, \quad t > 0; \quad (2a)$$

$$\left[\kappa \frac{\partial \Delta T(x, t)}{\partial x} + h \Delta T(x, t) \right]_{x=L} = 0, \quad t > 0; \quad (3a)$$

and

$$\Delta T(x, 0) = T_0 - \bar{T} = \Delta T_0, \quad t = 0. \quad (4a)$$

Furthermore, it is assumed that, with no forced coolant flow initially and high-conductivity plates, the condition of complete plate boundary insulation with uniform internal heat generation is approximated for $t < 0$. The insulation is suddenly removed at $t = 0$, which, in turn, is expressible by letting $T(x, 0) = T_0$ be constant.

Once the temperature distribution is determined from the preceding differential equation, boundary and initial conditions, the thin-plate thermal stresses are assumed to satisfy.⁴⁴

$$\sigma = \frac{\alpha E}{1 - \nu} \left\{ -T + \frac{1}{2L} \int_{-L}^L T \, dx + \frac{3x}{2L^3} \int_{-L}^L T x \, dx \right\}, \quad (5)$$

⁴⁴See Ref. 41, p. 278.

where

σ = normal stress parallel to plane of plate

α = coefficient of thermal expansion

E = Young's Modulus

ν = Poisson's Ratio.

In solving the system described by equations (1a) through (4a), the Laplace Transformation⁴⁵ method is used. The transform of a function (with respect to t) is indicated by a bar over the corresponding function designation. Accordingly, Eq. (1a) can be written as

$$\kappa \frac{d^2 \overline{\Delta T(x,p)}}{dx^2} - p \overline{\Delta T(x,p)} = -\overline{U(p)} \quad , \quad (6)$$

where

$$\overline{U(p)} = \frac{\overline{Q(p)}}{\rho c} + \Delta T_0 \quad . \quad (7)$$

The transformed boundary conditions, Eqs. (2a) and (3a), become

$$\left. \frac{d \overline{\Delta T(x,p)}}{dx} \right|_{x=0} = 0 \quad (8)$$

and

$$\left[\kappa \frac{d \overline{\Delta T(x,p)}}{dx} + h \overline{\Delta T(x,p)} \right]_{x=L} = 0 \quad . \quad (9)$$

The solution of Eq. (6) is

$$\overline{\Delta T(x,p)} = A e^{\sqrt{\frac{p}{\kappa}} x} + B e^{-\sqrt{\frac{p}{\kappa}} x} + \frac{\overline{U(p)}}{p} \quad , \quad (10)$$

where A and B may be functions of p .

Using Eqs. (8), (9) and (10), we find that

$$A = B = - \frac{h \overline{U(p)}}{p \left[\kappa \sqrt{\frac{p}{\kappa}} \sinh \sqrt{\frac{p}{\kappa}} L + h \cosh \sqrt{\frac{p}{\kappa}} L \right]} \quad , \quad (11)$$

⁴⁵Jaeger, J. C., Laplace Transformation, Methuen Monograph.

and the transform of $\Delta T(x,t)$ becomes

$$\overline{\Delta T(x,p)} = \frac{\overline{U(p)}}{p} \left[1 - \frac{h \cosh \sqrt{\frac{p}{\kappa}} x}{k \sqrt{\frac{p}{\kappa}} \sinh \sqrt{\frac{p}{\kappa}} L + h \cosh \sqrt{\frac{p}{\kappa}} L} \right] . \quad (12)$$

If we let

$$\frac{h \cosh \sqrt{\frac{p}{\kappa}} x}{p \left[k \sqrt{\frac{p}{\kappa}} \sinh \sqrt{\frac{p}{\kappa}} L + h \cosh \sqrt{\frac{p}{\kappa}} L \right]} = \overline{V(x,p)} , \quad (13)$$

we then want to obtain

$$\Delta T(x,t) = \mathfrak{L}^{-1}[\overline{\Delta T(x,p)}] = \mathfrak{L}^{-1} \left[\frac{\overline{U(p)}}{p} \right] - \mathfrak{L}^{-1} [\overline{U(p)} \overline{V(x,p)}] , \quad (14)$$

where

$$\mathfrak{L}^{-1} \left[\frac{\overline{U(p)}}{p} \right] = \mathfrak{L}^{-1} \left[\frac{\overline{Q(p)}}{p \rho c} + \frac{\Delta T_0}{p} \right] = \int_0^t \frac{Q(\tau)}{\rho c} d\tau + \Delta T_0$$

and

$$\mathfrak{L}^{-1} [\overline{U(p)} \overline{V(x,p)}] = \int_0^t U(t-\tau) V(x,\tau) d\tau = \int_0^t U(\tau) V(x,t-\tau) d\tau .$$

Now, note that, if $\phi(p) = g(p)/g(p)$, with p_j , the zeros of $g(p)$, all different, then

$$\phi(t) = \sum_{j=1}^{\infty} \frac{f(p_j)}{g'(p_j)} e^{p_j t} ,$$

where

$$g'(p) = \frac{dg(p)}{dp} .$$

Therefore, we find that

$$V(x,t) = \mathcal{L}^{-1} [\overline{V(x,p)}]$$

$$= \sum_{j=1}^{\infty} \frac{h \cosh \left(\sqrt{\frac{p_j}{\kappa}} x \right) e^{p_j t}}{\left(\frac{kLp_j}{2\kappa} + h \right) \cosh \sqrt{\frac{p_j}{\kappa}} L + \frac{1}{2} \sqrt{\frac{p_j}{\kappa}} (3k + h L) \sinh \sqrt{\frac{p_j}{\kappa}} L}, \quad (15)$$

where p_j ($j = 1, 2, 3, \dots$) are the solutions of

$$p \left[k \sqrt{\frac{p}{\kappa}} \sinh \sqrt{\frac{p}{\kappa}} L + h \cosh \sqrt{\frac{p}{\kappa}} L \right] = 0 \quad . \quad (16)$$

One obvious root of Eq. (16) is $p = 0$, say

$$p_1 = 0 \quad . \quad (17)$$

It remains to find the other values of p satisfying (16). To this end, set

$$\sqrt{\frac{p}{\kappa}} L = a + bi \quad ; \quad a \text{ and } b \text{ are real.} \quad (18)$$

Using Eqs. (16), (17) and (18), we obtain

$$k \left(\frac{a + bi}{L} \right) \sinh (a + bi) = h \cosh (a + bi) = 0 \quad , \quad (19)$$

from which can be written

$$\begin{aligned} & a \sinh a \cos b - b \cosh a \sin b + \frac{hL}{k} \cosh a \cos b \\ & + i (b \sinh a \cos b + a \cosh a \sin b + \frac{hL}{k} \sinh a \sin b) = 0 \quad . \end{aligned} \quad (20)$$

Therefore, a and b must satisfy the following simultaneous equations:

$$\left. \begin{aligned} a \sinh a \cos b - b \cosh a \sin b + \frac{hL}{k} \cosh a \cos b &= 0 \\ b \sinh a \cos b + a \cosh a \sin b + \frac{hL}{k} \sinh a \sin b &= 0 \end{aligned} \right\} \quad . \quad (21)$$

Equations (21) are satisfied if

$$\left. \begin{aligned} a &= 0 \\ b \tan b &= \frac{hL}{k} \end{aligned} \right\} \quad . \quad (22)$$

It can be shown that equations (22) provide all the required roots by obtaining a contradiction with the assumption that $a \neq 0$.

Then, noting that $b_n \tan b_n = hL/k$ except for $b = 0$, and using the notation $m = hL/k$, we can rewrite equations (15) as

$$V(x,t) = 1 - 2 \sum_{n=1}^{\infty} \frac{\cos \frac{b_n x}{L} e^{-\kappa b_n^2 t / L^2}}{\cos b_n \left(1 + m + \frac{b_n^2}{m} \right)} \quad (23)$$

Using these results in equation (14), we finally obtain

$$\Delta T(x,t) = 2m \Delta T_0 \sum_{n=1}^{\infty} \frac{\sin b_n \cos \frac{b_n x}{L} e^{-\kappa b_n^2 t / L^2}}{b_n (\sin^2 b_n + m)} \quad (24)$$

$$+ 2m \int_0^t \frac{Q(\tau)}{\rho c} \sum_{n=1}^{\infty} \frac{\sin b_n \cos \frac{b_n x}{L} e^{-\kappa b_n^2 (t - \tau) / L^2}}{b_n (\sin^2 b_n + m)} d\tau \quad .$$

Notice, from Eq. (24), that if $Q(\tau) = 0$, we have the solution to the problem in transient conduction without heat generation, in agreement with the solution (Eq. 7.2.569) in Boley and Weiner.⁴⁶

It is observed further from Eq. (24) that for $t = 0$,

$$2m \sum_{n=1}^{\infty} \frac{\sin b_n \cos \frac{b_n x}{L}}{b_n (\sin^2 b_n + m)} = 1 \quad (25)$$

Further examination of the implications of Eq. (25) reveals the possibility of expanding initial temperature distributions in the plate in terms of the infinite set $\{\cos(b_n x/L)\}$, where $b_n \tan b_n = m$, since then $\{\cos(b_n x/L)\}$ is an orthogonal set. However, it turns out that this set is not complete, and only temperature distributions that are even functions of x can be expanded as

⁴⁶See Ref. 41, Ch. 7.

$$\Delta T(x, 0) = \sum_{n=1}^{\infty} A_n \cos (b_n x/L) \quad . \quad (26)$$

This is not a serious handicap in many cases because of the symmetry frequently assumed about the plate midplane. Therefore, should it be desired later, it would not be necessary to assume $\Delta T(x, 0) = T_0$, a constant.

Under the conditions of symmetry being worked with here, it may be noted that Eq. (5) can be reduced to

$$\sigma = \frac{\alpha E}{1 - \nu} \left\{ -\Delta T(x, t) + \frac{1}{L} \int_0^L \Delta T(x, t) dx \right\} \quad . \quad (27)$$

By means of Eq. (24) in Eq. (27), Eq. (28) is obtained as

$$\begin{aligned} \frac{\sigma(1 - \nu)}{\alpha E(\Delta T_0)} = & \frac{m}{L} \int_{-L}^L \sum_{n=1}^{\infty} \frac{\sin b_n \cos b_n \frac{X}{L} e^{-\kappa b_n^2 t/L^2}}{b_n(\sin^2 b_n + m)} dx \\ & - 2m \sum_{n=1}^{\infty} \frac{\sin b_n \cos b_n \frac{X}{L} e^{-\kappa b_n^2 t/L^2}}{b_n(\sin^2 b_n + m)} \\ & + \frac{m}{L} \int_{-L}^L \left\{ \sum_{n=1}^{\infty} \frac{\sin b_n \cos b_n \frac{X}{L} e^{-\kappa b_n^2 t/L^2}}{b_n(\sin^2 b_n + m)} \int_0^t \frac{Q(\tau)}{\Delta T_0 \rho c} e^{-\kappa b_n^2 \tau/L^2} d\tau \right\} dx \\ & - 2m \sum_{n=1}^{\infty} \frac{\sin b_n \cos b_n \frac{X}{L} e^{-\kappa b_n^2 t/L^2}}{b_n(\sin^2 b_n + m)} \int_0^t \frac{Q(\tau)}{\Delta T_0 \rho c} e^{-\kappa b_n^2 \tau/L^2} d\tau \end{aligned} \quad (28)$$

Equation (28) is not written in some obviously more condensed form simply to aid in identifying some of the terms. For example, for $Q(\tau) = 0$, we have the transient stress condition with no internal heat generation, and the result for $x = L$ [the first two terms on the right-hand side of Eq. (28)] is plotted, for various values of m , on p. 284 in Boley and Weiner.⁴¹ For convenience, the set of curves through $m = 2$, taken from Boley and Weiner, is attached (Fig. VIII-1).

Fig. VIII-I. Thermal Stresses at the Surface of a Free Plate Heated Symmetrically, through a Boundary Conductance h , on the Faces $x = \pm L$. Initial temperature difference between plate surface and ambient ΔT_0 , Biot number $m = hL/k$. Note that surface stress is compressive for heating ($\Delta T_0 < 0$) and tensile for cooling ($\Delta T_0 > 0$). (From V. Paschkis, H. G. Landau, and J. H. Hlinka, Charts on Elastic Thermal Stresses in Heating and Cooling of Slabs and Cylinders, ASME Paper No. 57A238, 1957).

In order to consider the influence of allowable stress on limiting (for example) the heat generation function during startup, it would be necessary to program Eq. (28) for computer solutions. Further generalizing can also be accomplished, as pointed out earlier, for cases of nonuniform but symmetrical initial temperature distributions in the plate [see Eq. (26)].