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OPTIMIZATION OF THERMOELECTRIC GENERATORS FOR FIXED TEMPERATURE AND FIXED HEAT INPUT OPERATION

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by

Valvo Raag
RESALAB SCIENTIFIC
Menlo Park, California

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I. INTRODUCTION

In 1821, Thomas Johann Seebeck noted the deflection of a magnetic needle in the vicinity of a circuit composed of two dissimilar materials in a temperature gradient. Although he did not correctly interpret his observation, Seebeck is thus generally credited with the discovery of the thermoelectric effect, now bearing his name, in which a voltage is produced along a temperature gradient in a material. Thirteen years later, Jean Charles Athanase Peltier discovered that the passage of current across the juntion of two dissimilar materials resulted in heat generation or absorption at the juntion. Like Seebeck before him, Peltier failed to understand his discovery. It was several decades later that Lord Kelvin (William Thomson) established a relationship between the Seebeck and Peltier effects on the basis of thermodynamic arguments and predicted the existance of a third thermoelectric effect (the Thomson effect). The Thomson effect is characterized by the generation or absorption of heat in a homogeneous conductor with current flow in the direction of a temperature gradient. Even though Lord Kelvin therefore laid a theoretical foundation to thermoelectricity by relating the three thermoelectric effects in terms of thermodynamic principles, it was Altenkirch in 1909 and 1911 who developed the basic theory of thermoelectric power generation and cooling. Altenkirch determined that materials with high values of Seebeck coefficient and electrical conductivity and low values of thermal conductivity were needed for the practical utilization of thermoelectricity. Such materials, however, were not available in Altenkirch's days. As a result, the practical utilization of thermoelectric power generation and cooling remained essentially in the same state of dormancy in which they had been since the inception of thermoelectricity in 1821. It was only with the advent and wide scale use of semiconductors nearly fifty years later that suitable thermoelectric materials finally became available. It was in the 1950's therefore that thermoelectricity essentially underwent a rebirth, as manifested by the start of extensive theoretical, materials and device work in the United States and elsewhere.

Over the past fifteen or so years, along with the other mentioned work in thermoelectrics, considerable effort has been expended on the development of calculational techniques for the design and performance analysis of thermoelectric power generators. Much of this effort has involved the determination of generator configuration and load characteristics that optimize attainable performance. Because of considerable resultant mathematical simplification, the bulk of the optimization work has concentrated on thermoelectric power generating devices that operate under conditions of fixed hot and cold side operating temperatures. Inasmuch as most thermoelectric generators in reality operate under conditions of fixed heat input rather than fixed temperatures, the usual optimization procedures result in generator designs that therefore yield only approximately optimum performance. Nevertheless, the approximate fixed operating temperature treatments of thermoelectric generator design and performance analysis possess in some respects the simplicity and clarity that frequently is lost in the more rigorous handling of the problem. Therefore, although detailed design and analytical work in thermoelectrics should generally be based on treatments that consider fixed heat input generator operation, the approximate case of fixed temperature operation enables the key elements of the theory of thermoelectric power generation to be expounded in a relatively simple and straightforward manner. Unfortunately, however, it appears that the difference in the two modes of thermoelectric device operation is not universally appreciated and therefore it happens that the approximate theory is frequently used even in serious engineering work in thermoelectrics.

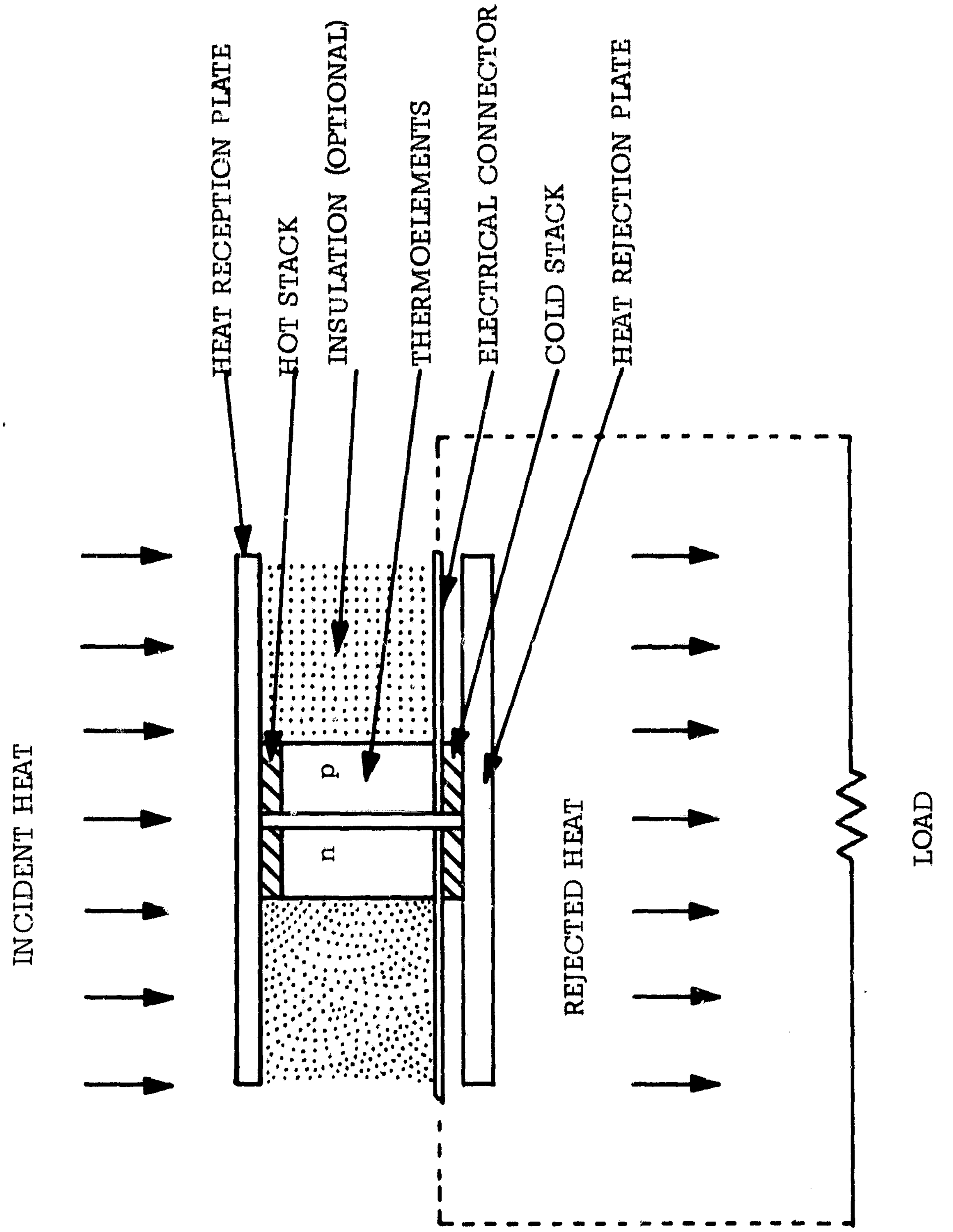
Because of the confusion that still, in some cases, exists on the optimization of thermoelectric devices for fixed temperature or fixed heat input operation, it is believed that an examination of certain areas of the problem may assist in clarifying the situation. It is the intent of the present exposition, therefore, to study certain key aspects of the optimization of thermoelectric devices for constant temperature as well as constant heat input operation and to point out the more important differences in the two cases.

II. THERMOELECTRIC POWER GENERATION

Thermoelectric power generating devices generally consist of one or more electrically interconnected thermocouples arranged around a suitable heat source. A typical thermocouple configuration is schematically illustrated in Figure 1. In addition to the active thermoelectric material, which normally consists of one n-type and one p-type leg, each thermocouple is comprised of extended area hot and cold side heat exchangers for the enhanced collection and rejection of heat at the two sides respectively and of so-called hot and cold stacks that connect the active material to the heat exchangers. The hot and cold stacks may include a variety of components such as pressure loading members, electrical insulators and stress alleviation disks. The void volume between the heat exchanger plates is usually filled with thermal insulation for the purpose of minimizing thermal shunt losses; it is obviously desirable to force as much of the incident heat as possible to pass through the active thermoelectric material.

A number of simplifying assumptions will now be made concerning the thermocouples in a thermoelectric generator in order to facilitate subsequent discussion. It will be assumed that all thermocouples in a device are identical and operate under identical conditions. This assumption amounts to the neglect of normal manufacturing variations as well as the practicalities of end and other effects that exists in an actual generator, and it enables the present treatment to be based on the performance of a single thermocouple rather than on the integrated total of more than one. Because the hot and cold stacks are only incidental, although necessary, members of a thermocouple, their effects on the performance of the thermocouple will be neglected. Similarly, the contribution of contacts, electrical interconnects and lead wires to the electrical resistance of the thermoelectric circuit which consists of the thermocouple and the external load, will be ignored. It will further be assumed that the temperature gradients associated with the thermocouple are

FIGURE 1.


HEAT RECEPTION PLATE
HOT STACK
INSULATION (OPTIONAL)
THERMOELEMENTS
ELECTRICAL CONNECTOR
COLD STACK
HEAT REJECTION PLATE
INCIDENT HEAT
p
n
REJECTED HEAT
LOAD

wholly axial, that the thermal insulation is a perfect insulator and that the heat exchanger members at the extremities of the thermocouple possess infinite thermal conductivities. The last two simplifications enable the assumption that all electrical resistance of the circuit resides wholly in the thermoelectric material and the external load, that no thermal shunt losses exist and that there are no temperature gradients in the direction transverse to that of primary heat flow.

Within the scope of the present discussion, none of these assumptions and simplifications have an important bearing on the conclusions to be formulated; they enable the attainment of considerable clarity and within the present context are therefore warranted. Needless to say, however, these assumptions are not necessary and should not be made in the design and performance analysis of an actual thermoelectric generator.

Heat incident on one side of the thermocouple shown in Figure 1 traverses the thermocouple and is rejected at the other side. As a consequence of the heat flow, a temperature difference, ΔT, is established across the thermocouple, where $\Delta T = T_H - T_C$, with T_H and T_C the resultant thermocouple hot and cold junction temperatures, respectively. The equation that describes this phenomenon may be written as

$$Q_K = K \Delta T, \qquad (1)$$

where Q_K pertains to the conducted heat and K represents the total conductance of the thermocouple. The conductance of the thermocouple is given by

$$K = \frac{1}{\ell} \left[A_n k_n + A_p k_p \right], \qquad (2)$$

where A and ℓ are the cross-sectional areas and length of the thermoelements and k is the thermal conductivity of the thermoelectric material. Subscripts n and p denote the n- and p-type thermoelectric materials used for the two legs of a thermocouple. Although not necessary, it is noted that both thermoelements, in view of common practice, have been assigned identical lengths.

The temperature difference across the thermocouple, established as a result of heat conduction, sets up voltages due to the Seebeck effect across the thermoelements. The voltages are additive because of the different polarities of the thermoelectric material in the two legs and the equilivant electrical circuit of the thermocouple (see Figure 1). The total voltage developed at the terminals of the thermocouple, E_o , may be written

$$E_o = S\Delta T, \tag{3}$$

where S is the combined Seebeck coefficient of the two thermoelements and is given by

$$S = S_p - S_n. \tag{4}$$

Subscripts n and p again denote the two types of thermoelectric material in the thermocouple. It should be noted that the so-called absolute Seebeck coefficient* values of n-type thermoelectric materials are negative and therefore the minus sign in Eq. (4) actually results in the addition of the absolute values of the absolute Seebeck coefficients of the n - and p-type thermoelectric materials of a thermocouple.

If a load of resistance R_L is now connected across the terminals of the thermocouple, the result will be the flow of current, I. By means of Ohm's law, the current may be expressed by

$$I = \frac{S\Delta T}{R + R_L}, \tag{5}$$

where R is the internal resistance of the thermocouple and is given by

$$R = \ell\left[\frac{\rho_n}{A_n} + \frac{\rho_p}{A_p}\right], \tag{6}$$

with ρ_n and ρ_p the electrical restivities of the n - and p-type thermoelectric materials respectively.

* - The absolute Seebeck coefficient of a material refers to its Seebeck coefficient as referenced to that of another material with zero Seebeck coefficient, such as a superconductor.

Three different physical properties of the n- and p-type thermoelectric materials have appeared in the above equations. These properties, are the thermal conductivity, the Seebeck coefficient and the electrical resistivity. The thermoelectric properties of most materials, as is the case with material characteristics in general, are temperature dependent functions. Because a thermocouple operates over a variety of temperatures, in the range T_H to T_C, the values assumed for the thermoelectric properties in Egs. (2), (4) and (6) must therefore be suitably averaged over the operating temperatures. A general equation for the averaging may be defined as follows[1]

$$\xi = \frac{\int_{T_C}^{T_H} \xi(T)dT}{\int_{T_C}^{T_H} dT}, \tag{7}$$

where ξ represents the property of which the average is desired. Thus ξ applies equally to k_n, k_p, S_n and S_p. It also applies to μ, the Thomson coefficient, which will be introduced below. As pointed out by Heikes and Ure[2], the average electrical resistivity, however, is more appropriately defined by

$$\rho = \frac{\int_{T_C}^{T_H} \rho(T)\, k(T)\, dT}{\int_{T_C}^{T_H} k(T)\, dT}, \tag{8}$$

because under open-circuit operating conditions it results in correct values of internal resistance, thermal conductance and voltage.

Up to this point, therefore, it has been seen that the heat conducted through the thermocouple establishes a temperature gradient across it which, as a result of the Seebeck effect, sets up a voltage across the thermoelements. Attachment of a load to the thermocouple terminals results in current flow through the circuit. The current flow across the various interfaces between dissimilar materials in the circuit, however, results in heat generation or absorption as a result of the Peltier effect. The quantity of heat Q_P, thus generated (absorbed) is given by the product of current I and Peltier coefficient π:

$$Q_P = I\pi, \tag{9}$$

where the Peltier coefficient is defined in terms of the Seebeck coefficient and temperature as

$$\pi = S(T)T. \tag{10}$$

The Seebeck coefficient value in Eq. (10) pertains to that at the temperature T of the junction to which Eq. (10) is applied. Thus, for example, the heat absorbed at the hot junction of a thermocouple is given by $(Q_P)_H = IS_H T_H$, where S_H represents the combined Seebeck coefficient values of the n - and p-type thermoelectric materials (see Eq. (4)) at the hot junction temperature T_H. The corresponding relationship for heat liberated at the cold junction of the thermocouple is $(Q_P)_C = IS_C T_C$. Whether heat is liberated or absorbed at a junction between dissimilar materials depends on the thermoelement polarity and the relative directions of current flow and temperature gradient. As indicated, heat is generally absorbed at the hot junction and liberated at the cold junction in power generating thermocouples.

In addition to the generation (absorption) of heat at the thermocouple junctions as a result of the Peltier effect, heat is also generated (absorbed) upon current flow in the thermoelements themselves because of the Thomson effect. The Thomson effect may be considered a differential Peltier effect in that it arises in materials which possess a temperature dependent Seebeck coefficient. Such materials operating in a temperature gradient have different values of Seebeck coefficient at each point in the material. Adjacent differential segments of such materials are therefore thermodynamically equivalent to dissimilar materials joined together. At each "interface", all along the length of the material, heat is liberated (absorbed) as a result of the Peltier effect. The total amount of heat liberated (absorbed) is obtained by integration along the length of the material and is called the Thomson heat, Q_T. The mathematical relationship that describes this phenomenon is written as

$$Q_T = I\mu\Delta T, \tag{11}$$

where μ is the net Thomson coefficient and is given by $\mu = \tau_p - \tau_n$ in terms of the Thomson coefficients of the individual n- and p-type thermoelements. The definition of τ for both type thermoelements is

$$\tau_i = T \frac{dS_i}{dT} , \tag{12}$$

where the subscript i pertains either to the n- or to the p-type thermoelement.

Current flow in conductors causes one additional heating effect, the so-called Joule heating that results from the finite resistance that all normal materials exhibit to current flow. The amount of Joule heat, Q_J, generated in the thermocouple may thus be written as

$$Q_J = I^2 R \quad . \tag{13}$$

In order to establish the precise operating characteristics of a thermocouple it is necessary to perform a detailed heat balance. In view of the four separate heating effects just discussed, it is necessary to relate these heat terms to the total heat incident on the thermocouple. The heat conducted through the thermocouple and the heat absorbed at the hot junction as a result of the Peltier effect must be directly supplied by the incident heat. The heat generated in the thermoelements by the Joule and Thomson effects undergoes distribution by a conduction mechanism and therefore also must contribute to the heat balances at the hot and/or cold junctions of the thermocouple.

In Appendix A it will be shown that to the first approximation one-half of the Joule and one-half of the Thomson heat generated in the thermoelements is transported to each of the junctions, the hot and the cold junction. The proof of this for the Joule heat alone, with vanishing Thomson coefficient, is well known and has been frequently derived in the past. Cohen and Abeles[3] have shown that thermocouple performance characteristics may be accurately calculated, when compared to "exact" numerical analyses, when this assumption is also applied ad hoc to the Thomson heat. As far as is known, however, the stated distribution of Joule and Thomson heats in a thermocouple has not previously been mathematically demonstrated in the form given in Appendix A.

A detailed heat balance at the hot junction of the thermocouple may therefore be formulated as

$$Q_H = Q_K + (Q_P)_H - (1/2)Q_T - (1/2)Q_J \quad . \tag{14}$$

where Q_H is the total heat incident on the thermocouple. The corresponding relationship for the cold junction may be written

$$Q_C = Q_K + (Q_P)_C + (1/2)Q_T + (1/2)Q_J \quad , \tag{15}$$

where Q_C represents the total heat rejected at the cold junction. On the basis of energy conservation considerations, it is obvious that Q_H and Q_C must differ by the amount of electrical power P produced by the thermocouple in the external load:

$$Q_H - Q_C = P = I^2 R_L \quad . \tag{16}$$

The validity of Eq. (16) will be demonstrated in Appendix B.

It should be noted that the algebraic combination of the various heat terms in Eqs. (14) and (15) neglects higher order interaction terms and is strictly valid only in the limit of vanishingly small Joule and Thomson heats and when the electrical resistivity, thermal conductivity and Thomson coefficient are independent of temperature[4]. The former condition generally applies to thermocouples of practical interest and the latter is approximately validated through the use of averaged thermoelectric property values. In general, conduction heat comprises some seventy percent of the total heat traversing a typical thermocouple used in power conversion applications. Peltier heat makes up the bulk of the remainder of the total heat, with Joule and Thomson heats contributing only a few percent each. The simplification inherent in Eqs. (14) and (15) enables at a minimum sacrifice to accuracy the solution of the thermoelectric power conversion problem; without this simplification, the problem would be quite intractable.

The algebraic signs exhibited for the various heat terms in Eqs. (14) and (15) are consistent with the above discussion on heat distribution in a thermocouple. According to the presently adopted convention, all positive signs refer to heat flow down the temperature gradient from the hot to the cold junction. Negative signs refer to heat flow in the opposite direction. The absorption of Peltier heat at the hot junction and liberation at the cold junction is equivalent to a flow down the temperature gradient.

To complete the general discussion on thermoelectric power generation, it is also important to consider the conversion efficiency of a generator. The conversion efficiency η is defined as the quotient of the electrical power output and the total heat input:

$$\eta = \frac{I^2 R_L}{Q_K + (Q_P)_H - (1/2)\, Q_T - (1/2) Q_J} . \qquad (17)$$

It should be remembered that Eq. (17), in view of the assumptions made earlier, represents an idealized efficiency, that due to the thermoelectric material itself. In an actual thermoelectric generator there exist numerous electrical and thermal losses, all of which detract from the ideal efficiency. Eq. (17) therefore represents the upper limit on conversion efficiency obtainable from a thermoelectric generator.

III. OPTIMUM THERMOELECTRIC PERFORMANCE

For direct or indirect economic reasons it is generally desirable to design a thermoelectric generator for optimum performance operation. From the equations exhibited in the preceding section it is apparent that the performance of a thermoelectric generator depends on a number of factors, such as generator operating temperatures, the thermoelectric properties of the material used, thermocouple configuration and generator load characteristics.

Because many of these factors depend on considerations related to the total power system design, such as the heat source and the heat rejection system, it is normally not possible to perform a detailed optimization of thermoelectric generator performance without treating the whole system. There is one type of optimization, however, and an important one, that may be performed nearly independently of the total system. This optimization pertains to the conversion efficiency and power output of the generator for any given values of the thermoelectric material properties and hot and cold side operating temperatures. Conversion efficiency optimization assumes special importance because of the high cost of fuels, such as nuclear fuels, that frequently are used in connection with the thermoelectric power conversion devices. For reasons of its economic importance and of its relative independence of detailed system design, considerable attention has therefore been devoted to thermoelectric generator efficiency optimization with respect to thermocouple configuration and generator load characteristics. As discussed in the Introduction, however, most of this effort has assumed fixed hot and cold side generator operating temperatures, rather than fixed heat input to the generator, and thus does not really represent the method of operation of most actual thermoelectric generators. It is the intent of the present section, therefore, to examine optimum generator performance under fixed operating temperatures as well as fixed heat input and to note the differences in the two cases.

It must be emphasized again, however, that the present treatment is only approximate in view of the simplifying assumptions made at the beginning of Section II. Moreover, the additional assumption that conversion efficiency may be optimized independently of the total system, although reasonable, is strictly not rigorous. Nevertheless, these same assumptions have formed the basis of nearly all thermoelectric optimization studies performed in the past and do enable the convenient discussion of the subject. In an actual thermoelectric generator design of course it is not necessary to make any of these assumptions and for enhanced accuracy, they should not be made.

FIXED TEMPERATURE PERFORMANCE OPTIMIZATION

In order to optimize the performance of a thermoelectric generator within the stated context of the present treatment, it will be necessary to determine the external load and the configuration of the thermocouples that optimize power output and conversion efficiency. As before, the analysis will consider a single thermocouple.

Defining $m = R_L/R$, the ratio of load to internal electrical resistance, and using Eqs. (1), (9), and (13), Eq. (17) for conversion efficiency may be written as

$$\eta = \frac{\Delta T}{T_H} \frac{m}{\frac{KR}{S^2 T_H}(1+m)^2 + \frac{S_H}{S}(1+m) - \frac{\Delta T}{2T_H} - \frac{\mu \Delta T}{2ST_H}(1+m)} \quad . \tag{18}$$

where use has also been made of Eq. (5) for the current I. Inspection of Eq. (18) shows that, in addition to operating temperatures and thermoelectric properties, conversion efficiency depends on the ratio of thermocouple load to internal electrical resistance m and, through the KR product, on thermoelement dimensions. Maintaining fixed temperatures, consequently also fixed average values of thermoelectric properties, it is possible to optimize Eq. (18) with respect to m and KR. Performing the former optimization first, it is found after differentiation of Eq. (18) with respect to m and letting the derivative vanish that the optimum value of m, defined as m_o, is given by

$$m_o = \left[1 + \frac{S^2 \Delta T}{KR}\left(\frac{S_H}{S}\frac{T_H}{\Delta T} - 1/2 - \frac{\mu}{2S}\right)\right]^{1/2} . \tag{19}$$

The substitution of Eq. (19) in Eq. (18) and the simplification of the resultant relationship yields

$$\eta = \frac{m_o - 1}{\left(\frac{T_H S_H}{S \Delta T} - \frac{\mu}{2S}\right)\left(m_o + 1\right) - 1} \quad , \tag{20}$$

for the conversion efficiency of a thermocouple in terms of the optimum ratio of load to internal electrical resistance. Because conversion efficiency depends on the inverse of the KR term (Eq. (19)), it is necessary to minimize the KR in order that efficiency be maximized[5]. The product KR, by means of Eqs. (2) and (6), is given by

$$KR = k_n \rho_n + k_n \rho_p \left(\frac{A_n}{A_p}\right) + k_p \rho_n \left(\frac{A_p}{A_n}\right) + k_p \rho_p \ . \tag{21}$$

After the differentiation of Eq. (21) with respect to (A_n/A_p), it is found that KR attains a minimum when

$$\frac{A_n}{A_p} = \left[\frac{\rho_n}{\rho_p} \cdot \frac{k_p}{k_n}\right]^{1/2} \ . \tag{22}$$

Equation (22) thus indicates the necessary relative ratio of the cross-sectional areas of the n- and p-type thermoelements of a thermocouple for maximizing conversion efficiency in fixed temperature operation. Substitution of Eq. (22) in Eq. (21) indicates that the minimum value of KR, defined as $(KR)_o$, is given by

$$(KR)_o = \left[\left(\rho_n k_n\right)^{1/2} + \left(\rho_p k_p\right)^{1/2}\right]^2 \ . \tag{23}$$

The substitution of Eq. (23) in the expression for the optimum ratio of load to internal electrical resistance, Eq.(19), yields

$$m_o = \left[1 + Z\Delta T\Gamma\right]^{1/2} , \tag{24}$$

where Z is defined as

$$Z = \frac{S^2}{\left[\left(\rho_n k_n\right)^{1/2} + \left(\rho_p k_p\right)^{1/2}\right]^2} , \tag{25}$$

and Γ is given by

$$\Gamma = \frac{2T_H S_H - \left(\mu + S\right) \Delta T}{2S\Delta T} \ . \tag{26}$$

The term $\mu\Delta T$ in Eq. (26) may be written as (see Appendix B)

$$\mu \Delta T = T_H S_H - T_C S_C - S\Delta T \ , \tag{27}$$

which upon substitution in Eq. (26) yields

$$\Gamma = \frac{T_H S_H + T_C S_C}{2S\Delta T} \ . \tag{28}$$

After the substitution of Eq. (24) in Eq. (20), the expression for optimum efficiency finally becomes

$$\eta_o = \frac{m_o - 1}{m_o (\Gamma + 1/2) - (\Gamma - 1/2)} \ . \tag{29}$$

The remaining performance parameters for the fixed temperature generator operating at optimum conversion efficiency may be written immediately on the basis of the above development and the pertinent equations of Section II. Thus, the load voltage V_L is given by

$$V_L = \frac{m_o S\Delta T}{m_o + 1} \ . \tag{30}$$

The current I is

$$I = \frac{S\Delta T}{(m_o + 1) R} \ , \tag{31}$$

and the power output P may be written as

$$P = \frac{m_o S^2 \Delta T^2}{(m_o + 1)^2 R} \ . \tag{32}$$

It is interesting to note that Eq. (29) was first derived by Cohen and Abels[3] on the basis of differential equations that describe heat flow in a thermocouple. As has just been demonstrated, the description of the heat balance in a thermocouple by means of algebraic equations (Eqs. (14) and (15)) yields the identical result in a vastly simplified manner.

The above treatment included the Thomson heat in the net heat balance of the thermocouple. In view of the definition of the Thomson coefficient (Eq. (12)), this implies that the treatment has accounted for the temperature dependence of the thermoelectric properties. It is more common, however, for reasons of simplicity, to neglect this temperature dependence of the thermoelectric properties and thereby eliminate the Thomson heat term from the net heat balance. The error produced in this way is only of the order of a few percent at most and this particular simplification is therefore very frequently made. Letting the Thomson coefficient μ vanish implies that the Seebeck coefficient is independent of temperature and S_H and S_C in Eq. (28) are the same as S. Making this simplification, it is possible to rewrite Eq. (29) as

$$\eta_o = \frac{\Delta T}{T_H} \cdot \frac{m_o - 1}{m_o + T_C/T_H} \tag{33}$$

where m_o is now given by

$$m_o = \left[1 + Z\bar{T}\right]^{1/2} , \tag{34}$$

with $\bar{T}$, the average temperature, defined as $\bar{T} = (T_H + T_C)/2$. Equation (33) is the equation that is commonly associated[5] with the optimum efficiency of a fixed operating temperature thermoelectric device. Inasmuch as Eq. (33) is not much simpler than the more complete Eq. (29), it is felt that the simplification obtained by neglecting Thomson heat generation (absorption) in the legs of a thermocouple is not really justified.

The optimum power output of a thermocouple under conditions of fixed operating temperatures is obtained by differentiating the equation for power output with respect to m, the ratio of load to internal thermocouple resistance. This operation is straightforward and simply indicates that maximum power output P_o occurs for the case in which load and internal electrical resistances are equal (matched load). Thus, the maximum power output of a thermocouple under fixed temperature operating conditions is given by

$$P_o = \frac{S^2 \Delta T^2}{4R} \quad . \tag{35}$$

Inspection of Eq. (24) for the ratio of load to thermocouple internal resistance at maximum conversion efficiency, however, indicates that for maximum efficiency the ratio is always greater than unity. In fact, for typical thermocouples and operating temperatures, it is usually found that efficiency maximizes for m values of the order of 1.2 to 1.3. Under fixed operating temperatures, therefore, the conversion efficiency and power output of a thermocouple maximize for different values of the ratio of load to internal resistance. Whereas this is true for thermoelectric devices operating at fixed temperatures, it is not true for devices that operate at fixed heat input. A little reflection will show that in the latter case, by definition, the power output and efficiency optimize for the same value of the ratio of load to internal resistance, a value that will be seen to differ from both of those derived for the case of thermoelectric device operation at fixed operating temperatures. On this very point, however, there appears to be considerable confusion and misunderstanding. Frequently[6] it is erroneously assumed that even in case of fixed heat input, a thermoelectric device produces maximum power when load and internal resistances are equal ($m = 1$). As trivial as the point may seem, and actually is, it must nevertheless be emphasized in view of the existing confusion that a thermocouple intended for operation with fixed heat input (such as obtained with radioisotope, fossil fuel, and solar heating) does not produce maximum power at matched load. Of course, in case of fixed operating temperature applications, power output and conversion efficiency do indeed optimize for different ratios of load to internal thermocouple resistance, as has been given by the above equations. Unfortunately applications for which this is true are relatively few. Operation with a nuclear reactor heat source, however, may be an application of this type.

For fixed temperature operation, thermocouple output power does not possess an optimum with respect to relative thermoelement dimensions. This is most conveniently seen from Eqs. (5) and (16). In general, however, for fixed operating temperatures, power output increases with decreasing thermoelement length and increasing cross-sectional area, i.e. power output increases with decreasing internal thermocouple resistance. This is intuitively obvious when considered in terms of heat transmitted through the thermocouple and conversion efficiency. The shorter and stubbier are the thermoelements, the more heat obviously passes through them. Conversion efficiency, however, is approximately proportional to the temperature difference across the thermocouple and nearly independent of thermocouple dimensions. For fixed operating temperatures, therefore, conversion efficiency is practically a constant and power output is directly proportional to the heat passing through the thermocouple; power output consequently increases with decreasing thermoelement length and increasing cross-sectional area.

Before concluding the discussion of thermocouple performance optimization in fixed temperature operation, attention is directed to Eq. (25) which defines the parameter Z. Because it is defined in terms of only the thermoelectric properties of the n- and p-type thermoelements and because it is approximately directly proportional to the maximum conversion efficiency of a thermocouple, Z serves as a convenient parameter for indicating the worth of combinations of n- and p-type materials in thermoelectric energy conversion applications. For this reason, Z, as defined by Eq. (25), is known as the "figure-of-merit" of a thermocouple. Inasmuch as the figure-of-merit defined by Eq. (25) pertains to the combination of two materials, an n-type and a p-type, it is sometimes convenient to consider the corresponding situation for a single material. The figure-of-merit of a single material, in analogy to Eq. (25), is therefore defined as

$$Z = \frac{S^2}{\rho k} \tag{36}$$

where the individual thermoelectric properties S, ρ and k pertain to either an n- or p-type material. The combination of the figures-of-merit of individual n- and p-type materials into the figure-of-merit of a thermocouple must make use of the following relationship

$$Z = \left[\frac{Z_n^{1/2} + \alpha Z_p^{1/2}}{1 + \alpha} \right]^2 \tag{37}$$

in order that consistency be obtained with Eq. (25). The parameter α is defined as

$$\alpha = \left[\frac{\rho_p k_p}{\rho_n k_n} \right]^{1/2} . \tag{38}$$

FIXED HEAT INPUT PERFORMANCE OPERATION

As in the case of fixed temperature operation, the performance of a thermoelectric generator in operation under conditions of fixed heat input will be considered from the standpoints of optimum load characteristics and thermocouple configuration. Not surprisingly, the results for the two cases will be found to considerably differ.

The conversion efficiency of a thermoelectric generator is defined as the quotient of the electrical power output and the heat input (see Eq. 17)). For the fixed heat input operation of a thermoelectric device, it is apparent from this definition that efficiency and power output are directly proportional to each other and that they both optimize for the same load characteristics and thermocouple configuration. For this reason, it therefore suffices for the case of fixed heat input operation of a thermoelectric device to optimize either the power output or the conversion efficiency in order to solve the whole problem.

Using Eqs. (5) and (16) and the definition $m = R_L/R$, the ratio of load to internal electrical resistance, the electrical power output P of a thermoelectric generator may be written as

$$P = \frac{mS^2 \Delta T^2}{R\,(1+m)^2} \; . \qquad (39)$$

Differentiating Eq. (39) with respect to m, without requiring ΔT to be fixed as in the case of fixed temperature operation, and letting the derivative vanish, it is found that the optimum ratio of load to internal electrical resistance m_o is given by

$$m_o = \frac{1-\beta}{2\beta} \left\{ 1 - \left[1 - \frac{4\beta}{(1-\beta)^2} \right]^{1/2} \right\} \qquad (40)$$

where β is defined in terms of ΔT and the derivative of ΔT with respect to m as

$$\beta = \frac{2}{\Delta T} \frac{d(\Delta T)}{dm} \; . \qquad (41)$$

It should be noted that the optimum ratio of load to internal resistance m_o approaches unity in the limit of vanishing β. A vanishing value of β of course implies the fixed temperature operation of a thermoelectric device and m_o of unity represents the optimum power output obtainable from a device operating under such conditions (see page 15).

Inspection of Eqs. (40) and (41) shows that in order to determine the optimum ratio of load to internal resistance m_o for a particular case, it will be necessary to know the appropriate value of $d(\Delta T)/dm$. The value of $d(\Delta T)/dm$ to be used is obtained from the total heat absorbed at the hot junction or rejected from the cold junction of the thermocouple, given by Eqs. (14) and (15). Using the former of these equations, after substitution of Eqs. (1), (5), (9) and (13), and solving for ΔT, it is found

$$\Delta T = \frac{b}{2a}\left[1-\left(1-\frac{4ac}{b^2}\right)^{1/2}\right], \tag{42}$$

where

$$a = \frac{S}{2R(1+m)^2}\left[S+\mu(1+m)\right], \tag{43}$$

$$b = K + \frac{SS_H T_H}{R(1+m)},$$

$$c = Q_H .$$

The differentiation of Eq. (42) with respect to m and the rearrangement of the result to conform with the definition of β in Eq. (41) yields

$$\frac{1}{\Delta T}\frac{d(\Delta T)}{dm} = \left[\frac{4ac}{Ab^2} - 1\right]\frac{1}{b}\frac{db}{dm} - \left[\frac{2ac}{Ab^2} - 1\right]\frac{1}{a}\frac{da}{dm}, \tag{44}$$

where

$$A = \left(1-\frac{4ac}{b^2}\right)^{1/2}\left[1-\left(1-\frac{4ac}{b^2}\right)^{1/2}\right], \tag{45}$$

and

$$\frac{1}{a}\frac{da}{dm} = \frac{1}{1+m}\left[\frac{\mu(1+m)+2S}{\mu(1+m)+S}\right], \tag{46}$$

$$\frac{1}{b}\frac{db}{dm} = \frac{\frac{1}{1+m} - \frac{1}{T_H}\frac{dT_H}{dm}}{\frac{KR(1+m)}{SS_H T_H} + 1} .$$

Equations (40) through (46) complete the problem of determining the optimum ratio of load to internal resistance m_o of a thermoelectric device operating under conditions of fixed heat input. Inspection of these equations may, at first glance, indicate a contradiction inasmuch as β, the parameter that determines m_o, depends, through Eqs. (43) to (46), itself on m. As may be expected, there of course is no contradiction and this curious result arises only because of a simplification that has implicitly been introduced into the present treatment. As stated above, the power output and conversion efficiency of a thermoelectric device operating under conditions of fixed heat input are directly proportional to each other. In determining the optimum ratio of load to internal resistance for a thermoelectric device operating in such a mode, it is therefore immaterial whether the optimization is performed in terms of conversion efficiency or in terms of power output - the final result in either case is the same. For convenience, it was decided in the present case to perform the optimization in terms of the power output, with the results as given above. Had the optimization been performed in terms of conversion efficiency, it would not have been possible to explicitly solve for the optimum ratio of load to internal resistance m_o, as given by Eq. (40), because the result would have been a fourth order equation in m_o. The solution of this equation for m_o would have necessitated numerical techniques. Although yielding the same results as the present treatment, expositional clarity would have been lost. The analysis of the problem in terms of power output optimization has enabled the display of the results in the form of the closed form equations given above. This method of analysis, however, has not really simplified the problem because of the apparently contradictory dependence of the optimum ratio of load to internal resistance on itself. Familiarity with the mathematics of simultaneous algebraic equations, on the other hand, shows the above treatment to be a classical case for the application of the method of successive approximations. It is this method therefore that enables the convenient determination of the optimum ratio of load to internal resistance in terms of the present treatment.

A fixed configuration and a fixed value of heat input Q_H are assumed for the thermocouple. The cold junction operating temperature of the thermocouple is either fixed at some desired value, the case of a heat sink of effectively infinite capacity, or is calculated by means of its dependence on the heat rejected at the cold side, the case, for example, of heat radiated into space. In the latter case, the first approximation cold junction temperature is determined by assuming that all of the heat incident on the thermocouple Q_H is rejected from the cold side; this assumption corresponds to that of assuming a vanishing conversion efficiency for the thermocouple. In higher order approximations this assumption is no longer necessary because the power output calculated for each approximation is used to determine the amount of heat rejected, and thus the cold side operating temperature, in the subsequent approximation. A value is also initially assumed for the hot junction temperature T_H of the thermocouple,(any reasonable value will do) because this is one of the variables that occurs in some of the equations that enter into the determination of m_o. Values of hot and cold junction temperatures are also needed for the establishment of appropriate thermoelectric properties needed in the calculation. As with the cold junction temperature, each approximation in the overall calculation yields a new hot junction temperature; this value of hot junction temperature is subsequently used in the following approximation. New values of thermoelectric properties, corresponding to the junction temperatures in question, are determined for each approximation. From the second of Eqs. (46) it is seen that for the calculation of m_o a value is also needed for dT_H/dm. Any reasonable value, such as zero, will suffice for the first approximation. Subsequent approximations may use $\Delta T\left[\left(1/\Delta T\right) d\left(\Delta T\right)/dm\right]$ as calculated in the approximation immediately preceding the one in question. If this is done, it is assumed that $d(\Delta T)/dm$ is equal to dT_H/dm. This assumption is more than adequate because of the relative smallness of the term involving dT_H/dm and because the cold junction temperature in most thermoelectric applications is a much more slowly varying function than the hot junction temperature.* Finally, an initial value is also needed for m. A value of unity may be used, although any other reasonable value is equally satisfactory.

The calculation of the optimum ratio of load to internal electrical resistance m_o is started by substituting the fixed and the initially assumed values of all pertinent parameters into Eqs. (43) and (46). The resultant values of a, b, c, $(1/a)da/dm$ and $(1/b)db/dm$ applied to Eqs. (41), (44) and (45) enable the first approximation determination of m_o by means of Eq. (40). At the same time, Eq. (42) permits the calculation of ΔT, which, along with the first approximation value of m_o substituted in Eq. (39), yields a value for the power output P. The total heat input to the thermocouple Q_H, lessened by this value of power output, enables the determination of the second approximation value of the cold junction temperature. The second approximation value of hot junction temperature follows immediately from the calculated values of cold junction temperature and the temperature differential ΔT. Substitution of the values thus derived for all pertinent parameters, including new values of thermoelectric properties and the first approximation value of m_o, into Eqs. (43) and (46) permits the start of the calculation for the next approximation. The process is repeated for as many approximations as is necessary to obtain desired convergence in the calculated value of m_o, i.e. until the value of m_o differs between two successive approximations by less than any desired amount. Convergence within less than one percent usually results after about three interations. As m_o converges to its optimum value, so do all of the other variables such as the junction temperatures, power output and consequently also the conversion efficiency.

* - See p.6 of Memorandum #2, prepared by V. Raag, RESALAB SCIENTIFIC, for JPL, July 30, 1969.

From the foregoing discussion of thermocouple performance optimization with respect to the ratio of load to internal electrical resistance it is seen that thermocouple operating temperatures are variable in the case of fixed heat input operation. This is analogous to the case of the fixed temperature operation of a thermocouple in which the heat input is variable, to be determined from the thermocouple configuration, thermoelectric properties and load characteristics by means of Eq. (14). Being variable, it may turn out that for an assumed configuration the hot junction temperature of the thermocouple at the optimum ratio of load to internal electrical resistance exceeds the limiting temperatures of the heat source or of the thermocouple itself. If that happens, it will be necessary to assume new configurations and repeat the optimization procedure until a configuration is found which enables performance optimization at permissible, or for that matter, at any desired operating temperature.

Thermocouple performance optimization in the case of fixed operating temperatures involved the determination of the optimum ratio of load to internal electrical resistance and of the relative cross-sectional areas of the n- and p-type thermoelements. Having just developed the formalism for the optimization of thermocouple performance with respect to load characteristics for the fixed heat input operating mode, it now remains to also consider the optimization with respect to the relative cross-sectional areas of the thermoelements. A theory nearly analogous to the one discussed above may also be developed for this latter optimization. The primary difference is that instead of m, the ratio of load to internal electrical resistance, the optimization parameter now is γ, the ratio of n- to p-type thermoelement cross-sectional areas. As explained above, in the fixed heat input operating mode the conversion efficiency and power output of a thermoelectric device are directly proportional and device performance may therefore be optimized with respect to either parameter; the results in both cases are identical. As before, for convenience it is power output that will be treated in the present instance. The usual maximizing procedure with respect to γ applied to Eq. (39) for power output yields the optimum γ, defined as γ_o, as follows

$$\gamma_c = \left\{\frac{\rho_n}{\rho_p} + \nu\left[\gamma\left(\gamma + 1\right)\left(\gamma + \frac{\rho_n}{\rho_p}\right)\right]\right\}^{1/2}, \tag{47}$$

where ν is defined by

$$\nu = \frac{2}{\Delta T}\frac{d(\Delta T)}{d\gamma}. \tag{48}$$

It is noted in Eq. (47) that the dependent variable γ also occurs as an independent variable. It is thus apparent that the solution of Eq. (47) once again requires successive approximation techniques. Inspection of Eq. (47) shows that the relationship is cubic in γ. Although it is possible to solve such an equation explicitly, it is just as convenient to execute the solution iteratively, the method adopted here. In order to determine ν in Eq. (48), it is necessary to differentiate Eq. (42) with respect to γ. Doing this and rearranging the result to conform with the form of Eq. (48), it is found

$$\frac{1}{\Delta T}\frac{d(\Delta T)}{d\gamma} = \left[\frac{4ac}{Ab^2} - 1\right]\frac{1}{b}\frac{db}{d\gamma} - \left[\frac{2ac}{Ab^2} - 1\right]\frac{1}{a}\frac{da}{d\gamma}, \tag{49}$$

where all the terms have been previously defined. The derivatives of a and b with respect to γ may be written

$$\frac{1}{a}\frac{da}{d\gamma} = \frac{1}{\gamma(1+\gamma)}\left[\frac{\gamma^2\rho_p - \rho_n}{\gamma\rho_p + \rho_n}\right], \tag{50}$$

$$\frac{1}{b}\frac{db}{d\gamma} = \frac{\dfrac{SS_H T_H}{KR(1+m)}\left[\dfrac{1}{a}\dfrac{da}{d\gamma} - \dfrac{1}{T_H}\dfrac{dT_H}{d\gamma}\right] - \dfrac{1}{K}\dfrac{dK}{d\gamma}}{\dfrac{SS_H T_H}{KR(1+m)} + 1},$$

where once again, all terms have been previously defined. For present purposes, however, the electrical resistance R and thermal conductance K have been rewritten in a form slightly different from that of Eqs. (2) and (6):

$$R = \frac{\ell}{A_T} \frac{1+\gamma}{\gamma} \left[\rho_n + \gamma \rho_p \right], \quad (51)$$

$$K = \frac{A_T}{\ell} \frac{1}{1+\gamma} \left[\gamma k_n + k_p \right],$$

with A_T being the total thermoelement cross-sectional area $(A_T = A_n + A_p)$. The derivative of the thermal conductance K with respect to γ in the form it occurs in Eq. (50), is given by

$$\frac{1}{K} \frac{dK}{d\gamma} = \frac{1}{1+\gamma} \left[\frac{k_n - k_p}{\gamma k_n + k_p} \right]. \quad (52)$$

Equations (47) to (52) define the optimization of the relative cross-sectional areas of the n- and p-type thermoelements of a thermocouple. In the actual use of these equations, fixed values are assumed for ℓ, A_T, m and Q_H. The cold junction temperature of the thermocouple is either fixed, the case of a heat sink of infinite capacity, or is calculated by means of its dependence on the heat rejected at the cold side. In the latter case, a first approximation cold junction temperature is calculated by assuming that all of the heat absorbed by the thermocouple Q_H is rejected at the cold side; this corresponds to the assumption of a vanishing conversion efficiency. In each higher order approximation the power output calculated for the preceding approximation is used to determine the amount of heat rejected, this enabling a progressively more accurate determination of the cold side temperature as the calculation proceeds. The hot junction temperature of the thermocouple is initially set at some arbitrary albeit reasonable value. As with the cold junction temperature, accurate hot junction temperatures are generated by the calculational sequence. Thermoelectric property values are adjusted after each iteration to reflect the calculated hot and cold junction operating temperatures of the thermocouple. The value of $dT_H/d\gamma$ in the second of Eqs. (50) is initialized at zero. In subsequent approximations it suffices if $\Delta T \nu/2$ is used for it, the inherent assumption being that the cold junction temperature is a much more slowly varying function of γ than the hot junction temperature. If desired, a more accurate procedure, analogous to the one developed in the reference given on the bottom of page 24, may be used.

The calculation for the optimum ratio of n- and p-type thermoelement cross-sectional areas is started by assuming an initial value, such as unity, for γ. Substitution of this and all of the other fixed and initialized values of pertinent parameters in Eqs. (43), (45), (51) and (52) enables the calculation of $(1/a)da/d\gamma$ and $(1/b)db/d\gamma$ by means of Eqs. (50) and the subsequent determination of ν by means of Eqs. (49) and (48). The substitution of this first approximation value of ν, along with the initialized value of γ, in Eq. (47) yields the first approximation value of γ_o. Equation (42) yields the first approximation value of ΔT, which through the use of either a fixed or calculated value of cold junction temperature, enables the determination of the first approximation value of hot junction temperature. All first approximation values thus determined for key parameters are used in the next iteration for the calculation of second approximation values. The procedure is repeated until convergence within any desired degree is obtained between two successive approximations.

At the conclusion of the calculation it may be found that for the values of A_T and ℓ used, the hot junction temperature will not be at a desired value. If that is the case, the values of A_T and ℓ may be changed and the sequence repeated until desired operating temperatures result. The value of m used in the calculation is completely arbitrary and may assume any numerical value. In a complete optimization procedure, however, it may be desirable to use an optimum value of m determined by the optimization procedure previously discussed. In fact, in actual use the optimization procedures for m and γ should really be combined because the optima of the two quantities are interdependent. The combination is simply effected by starting the calculational sequence with Eq. (40) and carrying it through to Eq. (52) on each iteration. Essentially the same goal could have been accomplished by starting the overall optimization by the maximizing of power output as $\partial^2 P/\partial m \partial \gamma = 0$.

It is fairly apparent from the foregoing treatment that the optimum values of m and γ are different in the cases of fixed temperature and fixed heat input operation. Interestingly enough, however, the same optimum ratios of n- and p-type thermoelement cross-sectional areas result for the two operating modes if the thermal conductivities of the two leg materials are identical. In general, however, the optimum load and thermoelement configurational characteristics are distinctly dependent on thermocouple operating mode and the results for the two modes of operation should therefore not be mixed.

ILLUSTRATIVE EXAMPLES

The results of the preceding discussion on thermocouple performance optimization with respect to relative thermoelement configuration and load characteristics are best illustrated by means of concrete numerical examples. Considering first the optimization with respect to the ratio of load to internal electrical resistance m, a thermocouple is assumed with dimensions and hypothetical thermoelectric properties as follows:

Electrical resistivity,	n-type	4.0mΩ-cm
	p-type	2.0 "
Thermal conductivity,	n-type	0.05 watt/°K-cm
	p-type	0.05 "
Total Seebeck coefficient		500 μv/°K

Thermoelement length	2.0 cm
Thermoelement area, n-type	0.2 cm^2
p-type	0.2 "
Total heat input	10 watts
Cold junction temperature	400° K

For ease of computation it has been assumed that the thermoelectric properties are independent of temperature, the Thomson coefficient thus vanishes, and that the cold junction temperature is fixed at 400° K. Although not necessary, these assumptions enable the simplification of the calculation without affecting the conclusions to be drawn from the results.

Using the equations and calculational sequence detailed for the determination of the optimum ratio of load to internal electrical resistance for the fixed heat input operating mode of a thermocouple, it may be calculated in a straightforward, albeit tedious manner that for the thermocouple in question the optimum value of m_o is 1.30. This value of m_o, of course, corresponds to the optima of both the power output and the conversion efficiency. The corresponding hot junction temperature is calculated to be 1239° K. Using this hot junction temperature, along with the other pertinent parameters given in the above listing, it is calculated by means of Eq. (19) that for fixed temperature operation the conversion efficiency optimizes for m_o of 1.16. Also for fixed temperature operation, the optimum value of power output corresponds to a value of 1.00 for m_o. Because identical thermocouple dimensions, material properties and operating temperatures have been used for the case of fixed temperature and fixed heat input operation in this example, it should be realized that to each value of m_o there corresponds a slightly different value of total heat input Q_H. Whereas the heat input for the fixed heat input case was originally set at 10 watts (corresponding to the m_o value of 1.30), the value of Q_H at m_o of 1.16 is 10.1 watts and at m_o of

1.00 is 10.2 watts. If the heat input is maintained at the fixed value of 10 watts, the hot junction temperatures are slightly dependent on m_o: $T_H = 1239°K$ at $m_o = 1.30$, $T_H = 1234°K$ at $m_o = 1.16$ and $T_H = 1229°K$ at $m_o = 1.00$. The variations in heat input and hot junction temperature, however, are so slight in the two cases that the optimum values of m_o to the precision given are unaffected.

From this example it is seen that for a given thermocouple and its operating conditions (heat input or temperatures), it is the method of optimization that determines the optimum value of the ratio of load to internal electrical resistance m. It is erroneous therefore to use the fixed operating temperature optimization procedure in the case of a device operating under conditions of fixed heat input and vice versa. Because of the typically broad maxima in the thermoelectric device performance curves, however, fortunately the penalty for mixing the results of the two modes of operation is usually not excessive. Generally, the lower the current, the more closely the optima for the two types of operation agree. Conversely, in very high current devices, those with high values of incident heat flux and short and stubby thermoelements, the difference between the optima for fixed temperature and fixed heat input operation may become appreciable.

Some of the parameters in the listing used for determining optimum thermocouple load characteristics have been changed for the example of the optimization of relative thermoelement cross-sectional areas. A thermocouple has been assumed with dimensions and hypothetical thermoelectric properties as follows:

Electrical resistivity,	n-type	4.0mΩ-cm
	p-type	2.0 "
Thermal conductivity,	n-type	0.0375 watt/°K-cm
	p-type	0.0750 "
Total Seebeck coefficient		500 μv/°K

Thermoelement length	2.0 cm
Total thermoelement area	0.4 cm^2
Total heat input	10 watts
Cold junction temperature	400° K
Ratio of load to internal resistance	1.00

As before, it is noted that for ease of computation the thermoelectric properties are assumed to be independent of temperature and the cold junction temperature is fixed at 400° K.

Using the formalism developed above for the determination of the optimum ratio of n- and p-type thermoelement cross-sectional areas of a thermocouple, it may be calculated that for the case defined by the given parameters, the optimum value of γ_o is 2.85. Using the given values of electrical resistivity and thermal conductivity in Eq. (22), it is seen that for the fixed temperature operating mode the optimum value of γ_o is 2.00. The difference in the results for the two operating modes is appreciable. As mentioned above, the bigger the difference in the thermal conductivities of the n- and p-type thermoelements, the bigger is the difference in the optimum ratios of thermoelement cross-sectional areas for the two operating modes. The optimum area ratios become identical for the two cases in the limit of identical thermal conductivities of the thermocouple leg materials. Fortunately in most instances of practical interest, the thermal conductivities of the n- and p-type thermoelements do not differ as much as in the present illustration. Usually they are not identical however and for this reason care should be taken to use the correct optimization procedure in the design of an actual thermoelectric device.

It should be noted that in the present example the hot junction temperatures corresponding to the optimum thermocouple configurations for the fixed temperature and fixed heat input operating modes are different. The hot junction temperature in the former case may be calculated to be 1220° K. In the latter case it is 1273° K. If desired, the hot junction temperature for the fixed heat input case may be dropped to that for the fixed temperature case by increasing the total (combined n- and p-type) thermoelement cross-sectional area to a value greater than the assumed 0.4 cm^2. The effect of this on the optimum value of γ_o is minimal. Thus it will be found that even for identical operating temperatures the optimum ratio of n- and p-type thermoelement cross-sectional areas is a function of thermocouple operating mode.

SUMMARY

The present treatment of thermocouple performance optimization in terms of external load characteristics and relative n- and p-type thermoelement configurations has considered optimization procedures for the cases of fixed temperature and fixed heat input thermocouple operating modes. Whereas most of the results derived for the case of fixed temperature operation are well known and have been previously available, the corresponding results for the fixed heat input case are essentially new. As far as is known, the only previous reported work on thermocouple performance optimization for fixed heat input operation is that of Castro and Happ[7]. The overall approach used by these investigators is, however, different from that of the present treatment and, more importantly, Castro and Happ incorrectly conclude that the optimum ratio of relative thermoelement cross-sectional areas is identical for fixed temperature and fixed heat input operating modes. The present study shows that optimum thermocouple leg configuration and load characteristics are different for the fixed temperature and fixed heat input operating modes. Because of this, the impropriety of using, as is commonly done, the fixed operating temperature optimization procedures in the design of thermoelectric devices intended for operation at fixed heat input and vice versa is emphasized.

In addition to the detailed treatment of thermoelectric device optimization procedures, the present treatment in some instances takes a new and different look at the basic theory underlying thermoelectric energy conversion. The results derived in the Appendices as well as the method of derivation of Cohen and Abeles'[3] efficiency expression, Eq. (29), are considered novel.

APPENDIX A

In the heat balance equations of Section II, Eqs. (14) and (15), it was assumed that of Joule and Thomson heat generated in the legs of a thermocouple, one-half is transported to each of the junctions. The proof of this for the case of Joule heat alone, with negligible Thomson heat, is well documented.[8] Cohen and Abeles[3], on the basis of an ad hoc assumption, showed that good agreement with "exact" numerical calculations of thermocouple performance results if this assumption is also applied to Thomson heat. As far as is known, however, a proof that in the first approximation one-half of both Joule and Thomson heats are transported to each of the junctions of a thermocouple has not previously been mathematically developed in the form to be given below. Burshtein[4] has derived the same results in a different manner. As mentioned in Section II, it will be assumed that the thermal conductivity, electrical resistivity and the Thomson coefficient of the thermoelectric materials are independent of temperature. The use of temperature averaged property values validates the assumption.

The heat gain in a differential section dx of a thermoelement is

$$Q_{in} - Q_{out} = C_v A dx \frac{\partial T}{\partial t} , \qquad (A1)$$

where C_v and A are the specific heat and cross-sectional area of the thermoelement and T is the temperature. The heat input to the differential section dx may be written

$$Q_{in} = kA \left.\frac{\partial T}{\partial x}\right|_x + \frac{I^2 \rho}{A} dx + I\mu \frac{\partial T}{\partial x} dx , \qquad (A2)$$

where k, ρ and μ are the thermal conductivity, electrical resistivity and Thomson coefficient of the thermoelement and I is the current. The heat leaving the different section dx is given by

$$Q_{out} = kA \left.\frac{\partial T}{\partial x}\right|_{x + dx} . \qquad (A3)$$

The differential equation describing the equilibrum temperature distribution in the thermoelement is obtained by taking the difference of Eqs. (A2) and (A3) and letting dx and $\partial T/\partial t$ vanish:

$$kA \frac{d^2T}{dx^2} + I\mu \frac{dT}{dx} + \frac{I^2\rho}{A} = 0 \tag{A4}$$

The solution of Eq. (A4) with boundary conditions $T(\ell)=T_H$ and $T(o)=T_C$ is

$$T(x) = h_1 \exp\left(\frac{I\mu x}{kA}\right) - \frac{I\rho}{\mu A} x + h_2 \quad , \tag{A5}$$

where ℓ is the length of the thermoelements, and T_H and T_C refer to the hot and cold junction temperatures respectively. The integration constants h_1 and h_2 are given by

$$h_1 = \frac{\Delta T + IR/\mu}{\exp(I\mu/K) - 1} \quad , \tag{A6}$$

$$h_2 = - \frac{\left[T_H - T_C \exp(I\mu/K) + IR/\mu\right]}{\exp(I\mu/K) - 1} \quad ,$$

where the thermal conductance K, electrical resistance R and the temperature difference ΔT are defined as

$$K = \frac{kA}{\ell} ,$$

$$R = \frac{\rho \ell}{A} , \tag{A7}$$

$$\Delta T = T_H - T_C .$$

The maximum temperature in the thermoelement occurs at x_m and is found by maximizing Eq. (A5) by the usual method of differentiating with respect to x and letting the result vanish. Doing this it is found

$$x_m = \frac{-kA}{I\mu} \ln\left(\frac{\rho k}{\mu^2 h_1}\right) . \tag{A8}$$

The fraction of the total heat transferred to the hot junction is that portion generated in the thermoelement between the hot junction and the position x_m

of the maximum temperature. The fraction n of the total heat transferred to the hot junction is therefore

$$n = \frac{\ell - x_m}{\ell} = 1 + \frac{K}{I\mu} \ln\left\{\frac{\rho k}{\mu}\left[\frac{\exp(I\mu/K) - 1}{\mu\Delta T + IR}\right]\right\}. \tag{A9}$$

Expansion of the exponential term in Eq. (A9) enables the equation to be written as

$$n = 1 + \frac{K}{I\mu} \ln\left\{\left[\frac{IR}{(\mu\Delta T + IR)}\right]\left[1 - \frac{I\mu}{2K} + \frac{I^2\mu^2}{6K^2} - \cdots\right]\right\} \tag{A10}$$

Expressing the logarithm of the product of the bracketed terms in Eq. (A10) as the sum of the logarithms of each term individually and expanding each, it is found

$$n = 1 + \frac{K}{I\mu}\left\{\frac{-\mu\Delta T}{\mu\Delta T + IR}\left[1 + 1/2\left(\frac{\mu\Delta T}{\mu\Delta T + IR}\right) + 1/3\left(\frac{\mu\Delta T}{\mu\Delta T + IR}\right)^2 + \cdots\right]\right.$$

$$\left. - \frac{I\mu}{2K}\left(1 - \frac{I\mu}{3K} + \cdots\right)\left[1 + \frac{I\mu}{4K}\left(1 - \frac{I\mu}{3K} + \cdots\right) + \cdots\right]\right\} \tag{A11}$$

With the retention of only the first order terms in each of the expansions in Eq. (A11), it is possible to write a first approximation for n as

$$n = 1/2 - \frac{K\Delta T}{I\mu\Delta T + I^2R} . \tag{A12}$$

The total heat Q_H transferred to the hot junction is equal to the combination of heat absorbed at the junction by the Peltier effect and the heat transferred by the above process. Thus the heat balance at the hot junction may be written as

$$Q_H = IS_HT_H - n\left[I^2R + I\mu\Delta T\right], \tag{A13}$$

where S_H refers to the Seebeck coefficient of the thermoelement at the hot junction temperature T_H. Substitution of Eq. (A12) in Eq. (A13) finally yields

$$Q_H = K\Delta T + IS_HT_H - (1/2)I^2R - (1/2)I\mu\Delta T , \tag{A14}$$

which is identical to Eq. (14) in section II if S, μ , K and R in the present development are redefined to include both legs of a thermocouple, as they are in Section II. From Eq. (A14) it is seen that in the first approximation one-half of the Joule and Thomson heat generated in the legs of a thermocouple is transported to the hot junction. It is therefore trivially true that one-half of the Joule and Thomson heat generated is also transported to the cold junction of the thermocouple. This has been assumed in Eq. (15) of Section II. If desired, the proof for the fraction of heat delivered to the cold junction may be executed in a manner analogous to the one above for the hot junction.

It should be noted that the above derivation is based on the assumption of only a small temperature difference ΔT between the hot and cold junctions of a thermocouple because it has been assumed that the maximum temperature occurs between and not at the junctions. This same assumption also underlies the usual treatments of the problem in which only contributions due to Joule heating are taken into account. In thermoelectric power conversion applications to thermocouples with relatively large values of temperature difference, Eq. (A14) therefore neglects all terms of interaction between Joule, Thomson and conduction heat. The importance of such interaction terms cannot unfortunately be assessed from the relative magnitudes of the corresponding terms in Eq. (A11) because, as stated, the above derivation only strictly applies to thermocouples with small temperature differences. The use of the heat balance equations, Eqs. (14) and (15) in Section II, therefore implicitly assumes the independence of conduction heat and Joule and Thomson heats.

Finally, within the scope of the above derivation, the neglect or retention of higher order terms in the expansion of Eq. (A11) of course depends on the relative magnitude of the various arguments. Examination of a few higher order terms indicates that the Thomson heat term in Eq. (A14) may in fact in some cases be comparable in magnitude to the next terms in the expansion. In view of the comments about the basis of the above derivation, in such instances it may be appropriate to neglect all Thomson heat contributions.

APPENDIX B

In Section II it was stated that the electrical power delivered to the load of a thermoelectric generator may be assumed to be equal to the difference in the heat absorbed at the hot side and the heat rejected at the cold side of the generator. On the basis of energy conservation it is obvious that this assumption must be true. Nevertheless, it is instructive to prove its validity by means of direct calculation. As before, the proof will be based on a single thermocouple connected to a load. The generalization to any number of thermocouples is straightforward.

A detailed heat balance (see Section II) at the hot junction of the thermocouple may be written as

$$Q_H = Q_K + (Q_P)_H - 1/2\, Q_T - 1/2\, Q_J \,, \tag{B1}$$

where Q_H is the total heat incident on the thermocouple. The corresponding relationship for the cold junction may be written

$$Q_C = Q_K + (Q_P)_C + 1/2\, Q_T + 1/2\, Q_J \,, \tag{B2}$$

where Q_C represents the total heat rejected at the cold junction. All of the terms in Eqs. (B1) and (B2) have been defined in Section II. The difference of Eqs. (B1) and (B2) is

$$Q_H - Q_C = (Q_P)_H - (Q_P)_C - Q_T - Q_J \ . \tag{B3}$$

making use of Eqs. (9), (11) and (13), Eq. (B3) may be rewritten as

$$Q_H - Q_C = IS_H T_H - IS_C T_C - I\mu\Delta T - I^2 R \ . \tag{B4}$$

The use of Eq. (12) for the Thomson coefficients of the n- and p-type thermoelements enables μ to be defined as

$$\mu = T \frac{dS}{dT} \tag{B5}$$

The average value of μ, to be used in Eq. (11) and therefore also in Eq. (B4), is defined in terms of Eq. (7) as

$$\mu = \frac{\int_{T_C}^{T_H} T \frac{dS}{dT} dT}{\int_{T_C}^{T_H} dT} . \tag{B6}$$

The denominator of Eq. (B6) is simply ΔT; Eq. (B6) thus becomes

$$\mu \Delta T = \int_{T_C}^{T_H} TdS . \tag{B7}$$

Performing the indicated integration by parts, it is found

$$\int_{T_C}^{T_H} TdS = \left[ST\right]_{T_C}^{T_H} - \int_{T_C}^{T_H} SdT . \tag{B8}$$

The use of Eq. (7) for the definition of the average Seebeck coefficient enables Eq. (B8) to be rewritten as

$$\int_{T_C}^{T_H} TdS = S_H T_H - S_C T_C - S\Delta T , \tag{B9}$$

where the integration limits indicated in Eq. (B8) have been applied to the integrated term. Substitution of Eq. (B9) in Eq. (B7) and then in Eq. (B4) yields

$$Q_H - Q_C = IS\Delta T - I^2 R . \tag{B10}$$

Substitution of Eq. (5) in Eq. (B10) finally gives

$$Q_H - Q_C = I^2 R_L , \tag{B11}$$

which by definition is the power P_o delivered to the load of the thermocouple.

An interesting by-product of this demonstration is the clear indication of the close relationship between the three thermoelectric effects, viz. the Seebeck, Peltier and Thomson effects, that Thomson discovered over a hundred years ago. This relationship is explicitly exhibited by differentiating Eq. (10) with respect to temperature and making use of Eq. (B5):

$$\frac{d\pi}{dT} = S + \mu \quad . \tag{B12}$$

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