Design and Optimization of Compatible, Segmented Thermoelectric Generators

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Abstract

The thermoelectric compatibility factor is used to rationally select materials for a segmented thermoelectric generator. The thermoelectric potential is used for the exact analytic expressions for materials with temperature dependent thermoelectric properties. This calculation does not assume constant or averaged thermoelectric properties as is often done for analytic results. The calculations use the relative current density as the intensive independent variable. A method of optimizing the system configuration is outlined that allows a separation of the system level and thermoelectric level with only three interface parameters: thermoelectric hot side temperature, cold side temperature and the heat flux. The calculation of performance under non-optimal conditions is described.

Introduction

The efficiency of a thermoelectric generator is governed by the thermoelectric properties of the generator materials and the temperature drop across the generator. The temperature difference, ΔT between the hot side (T_h) and the cold side (T_c) sets the upper limit of efficiency through the Carnot efficiency $\eta_C = \frac{\Delta T}{T_H}$. The thermoelectric material governs how close the efficiency can be to Carnot primarily through the thermoelectric figure of merit, z, defined by

$$z = \frac{\alpha^2}{\kappa\rho} \tag{1}$$

The relevant materials properties are the Seebeck coefficient α, the thermal conductivity κ, and electrical resistivity ρ, which all vary with temperature. For a material with thermoelectric properties (α, ρ, κ) constant with respect to temperature the efficiency is given by

$$\eta = \frac{\Delta T}{T_h} \cdot \frac{\sqrt{1+z\overline{\overline{T}}}-1}{\sqrt{1+z\overline{\overline{T}}}+T_c/T_h} \tag{2}$$

Thus to achieve high efficiency, both large temperature differences and high figure of merit materials are desired. Since the material thermoelectric properties (α, ρ, κ) vary with temperature it is not desirable or even possible to use the same material throughout an entire, large temperature drop. Ideally, different materials can be *segmented* together such that a material with high efficiency at high temperature is segmented with a different material with high efficiency at low temperature. In this way both materials are operating only in their most efficient temperature range.

We have shown [1] that for the exact calculation of thermoelectric efficiency, the thermoelectric compatibility must also be considered. Compatibility is most important for segmented generators because the thermoelectric material properties may change dramatically from one segment to another. If the compatibility factor defined as

$$s = \frac{\sqrt{1+zT}-1}{\alpha T} \tag{3}$$

differs by about a factor 2 or more, both segments can not be simultaneously operating efficiently, and the overall efficiency will actually decrease.

The exact solution to the one dimensional thermoelectric problem is succinctly given by using the thermoelectric potential defined by [1]

$$\Phi = \alpha T + \frac{1}{u} \tag{4}$$

where u is the relative current density given by

$$u = \frac{J}{\kappa\nabla T} \tag{5}$$

Note that the current in the n-element is in the opposite direction as the p-element so that $I_n = -I_p$. Similarly, u_n and Φ_n are typically negative.

The heat transported Q is given by

$$Q = I\Phi \tag{6}$$

The voltage produced by the temperature difference with a current flow is

$$V = \Delta\Phi = \Phi_h - \Phi_c \tag{7}$$

Using only the relative current density $u(T)$ and temperature T as independent variables, the efficiency of a thermoelectric element is given by

$$\eta = \frac{\Delta\Phi}{\Phi} = 1 - \frac{\alpha_c T_c + \frac{1}{u_c}}{\alpha_h T_h + \frac{1}{u_h}} \tag{8}$$

The subscripts h and c denote the value at the thermoelectric hot or cold side (T_h = hot side temperature, $\alpha_h = \alpha(T_h)$)

To calculate the variation of $u(T)$ with temperature, the differential equation, derived from the heat equation, must be solved

$$\frac{d(1/u)}{dT} = -\frac{1}{u^2}\frac{du}{dT} = -T\frac{d\alpha}{dT} - u\rho\kappa \tag{9}$$

The efficiency of a thermoelectric generator can be computed from the individual efficiency of the n- and p-elements

$$\eta_{np} = \frac{\eta_p Q_p + \eta_n Q_n}{Q_p + Q_n} \quad (10)$$

The exact solution for the two element (n-type and p-type) is [2]

$$\eta = 1 - \frac{\alpha_{p,c} T_c + \frac{1}{u_{p,c}} - \alpha_{n,c} T_c - \frac{1}{u_{n,c}}}{\alpha_{p,h} T_h + \frac{1}{u_{p,h}} - \alpha_{n,h} T_h - \frac{1}{u_{n,h}}} \quad (11)$$

which can be optimized by varying initial u conditions for both n-type and p-type elements. The relative current u values will in general have a different magnitudes for n-type ($u < 0$) and p-type ($u > 0$) elements.

In this paper, we give a procedure for maximizing the efficiency for a segmented thermoelectric generator. We also describe a general method to design the thermoelectric generator to interface with the heat supply and sink.

Selection of Thermoelectric Materials

Since the efficiency of a thermoelectric generator is proportional to the Carnot factor, a large temperature difference is desired between the thermoelectric hot side and cold side. However, due to system design factors described below, the temperature difference across the thermoelectric generator is significantly less than that between the source and sink temperatures.

In this section, the highest efficiency thermoelectric generator materials are selected for *any thermoelectric hot side temperature* T_h *and cold side temperature,* T_c.

The maximum efficiency that a thermoelectric material can provide is determined by the thermoelectric figure of merit z. However, the maximum efficiency is only achieved when the relative current density u, is equal to the compatibility factor s [1]. In an efficient generator the relative current density is roughly a constant throughout a segmented element (typically u changes by less than 20%). Thus the goal is to select high figure of merit materials that have similar compatibility factors. If the compatibility factors differ by a factor of about two or more, a given u can not be suitable for both materials and segmentation will not be efficient. Other factors (not considered here) may also affect the selection such as: thermal and chemical stability, heat losses, coefficient of thermal expansion, processing requirements, availability and cost. For this analysis, we consider only the thermoelectric properties in the 1-dimenstional heat flow problem.

Selection of Interface Temperature

The optimum interface temperature between two segments can be estimated using the approximation that u remains constant within a thermoelectric leg [3]. The approximate interface is then the temperature where the reduced efficiency

$$\eta_r = \frac{u\frac{\alpha}{z}\left(1 - u\frac{\alpha}{z}\right)}{u\frac{\alpha}{z} + \frac{1}{zT}} \quad (12)$$

of one material crosses that of the other.

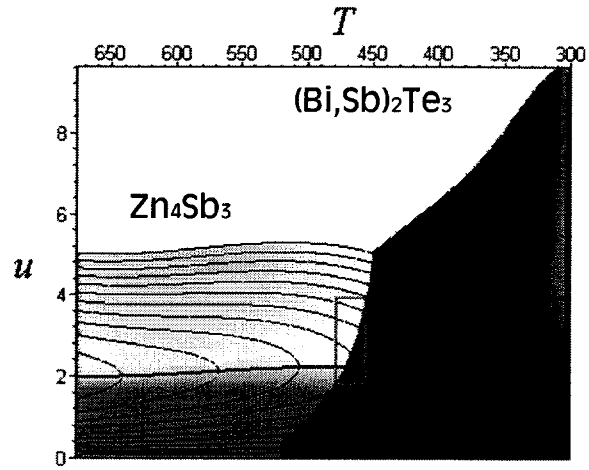

Figure 1: Contour surfaces of reduced efficiency as a function of u and T for p-type Zn_4Sb_3 and $(Bi,Sb)_2Te_3$. The line of $s(T)$ which is the value of u that would provide the highest reduced at a particular temperature is shown. The best interface temperature can be approximated by assuming u is a constant and finding the temperature where the efficiency surfaces cross. In this example the best interface T and u will be somewhere in the box indicated.

Once the interface temperatures are selected, the temperature variation of the thermoelectric properties ($\alpha(T)$, $\rho(T)$, $\kappa(T)$) for the entire element is defined under these optimum (u) conditions. The relative lengths of the segments are adjusted (described below) to achieve these interface temperatures (at a particular u value). In this way, the spatial variation of the properties ($\alpha(x,T)$ for example) need not be introduced: $\alpha(T) = \alpha(x(T),T)$ [4].

The exact optimum interface temperature can be computed with the exact calculation of efficiency. For this precision, commonly ignored simplifications such as heat losses, contact resistances, three-dimensional heat and current flow should be included.

Calculation of Efficiency

For computation, this can be approximated by combining the zero Thomson effect ($d\alpha/dT = 0$) solution with the zero resistance ($\rho\kappa = 0$) solution to equation (9), similar to [5].

$$\frac{1}{u_2} = \frac{1}{u_1}\sqrt{1 - 2u_1^2 \overline{\rho\kappa}\Delta T} - \overline{T}\Delta\alpha \quad (13)$$

where $\Delta\alpha = \alpha(T_2) - \alpha(T_1)$ and $\overline{\rho\kappa}$ denotes the average of $\rho\kappa$ between T_1 and T_2.

The above equation is also valid to calculate the change in u at the interface between segmented materials where α is discontinuous ($\Delta T = 0$, $\Delta\alpha \neq 0$).

Electrical and thermal contact resistance, both for the surface interface and the bulk resistivity of the contact, can be included as long as a budget for the temperature drop across the contact (ΔT) is allocated.

In this way, $u(T)$ can be calculated given an initial condition (either u_h or u_c). The maximum single element efficiency is found by varying these initial u conditions and calculating the efficiency from equation (11).

Requirements for Maximum Efficiency

The solution of maximum efficiency (equation 11) fixes the relative current density $u(T)$ in each element, the voltage and the ratio of the p- and n-type cross sectional area.

The voltage V produced is given by equation 7:

$$V = \left(\alpha_{p,h}T_h + \frac{1}{u_{p,h}} - \alpha_{n,h}T_h - \frac{1}{u_{n,h}}\right) - \left(\alpha_{p,c}T_c + \frac{1}{u_{p,c}} - \alpha_{n,c}T_c - \frac{1}{u_{n,c}}\right) \tag{14}$$

Integrating equation (5) [2, 6] gives

$$Jl = \int_{T_c}^{T_h} u\kappa dT \tag{15}$$

where l is the length of the element. Assuming the n-element and p-element have the same total length (and carry the same electrical current $\pm I$), the ratio of the cross sectional area of the p-element to the n-element, can be calculated from

$$\frac{A_p}{A_n} = \frac{-J_n}{J_p} = \frac{-\int_{T_c}^{T_h} u_n\kappa_n dT}{\int_{T_c}^{T_h} u_p\kappa_p dT} \tag{16}$$

The most efficient area ratio is then found from the most efficient $u_p(T)$ and $u_n(T)$.

In order to calculate l and further operating conditions, the total heat flux $Q_{total,h}/A_{total}$ or power/area desired P/A_{total} must be given. The power and heat input are related by the efficiency:

$$P = Q_{total}\eta \tag{17}$$

The current density J_p is calculated from

$$J_p = \frac{Q_{total,h}}{A_{total}} \times \frac{1 + \frac{A_n}{A_p}}{\Phi_{p,h} - \Phi_{n,h}} \tag{18}$$

where

$$\Phi_{p,h} - \Phi_{n,h} = \alpha_{p,h}T_h + \frac{1}{u_{p,h}} - \alpha_{n,h}T_h - \frac{1}{u_{n,h}} \tag{19}$$

The n-element current density, J_n, and l can then be calculated from equations 16 and 15.

Thus the power produced per cross sectional area is exactly inversely proportional to the length l:

$$P = \frac{A_{total}}{l} \times \Delta\Phi \frac{J_p l \times {}^{-}J_n l}{J_p l - J_n l} \tag{20}$$

or

$$P = \frac{A_{total}}{l} \times \Delta\Phi \frac{-\int_{T_c}^{T_h} u_p\kappa_p dT \times \int_{T_c}^{T_h} u_n\kappa_n dT}{\int_{T_c}^{T_h} u_p\kappa_p dT - \int_{T_c}^{T_h} u_n\kappa_n dT} \tag{21}$$

The terms $\Delta\Phi$, $J_p l$, $J_n l$ are fixed (by equations 14 and 15) once u_p and u_n are optimized for maximum efficiency. Thus any power density (P/A_{total}) can be achieved by adjusting l. Which means that in the "ideal" system [7] (with no thermal losses or electrical contact resistances) the maximum efficiency can always be achieved, making discussion of "maximum power density" unnecessary [8-10] for the "ideal" system.

The temperature variation along the length $l(T)$ (which may have different variation for n and p elements) can be calculated from equation (15):

$$l(T) = \frac{1}{J} \int_{T_c}^{T} u\kappa dT \tag{22}$$

Thermoelectric Converter Design

The system design given criteria may not be simply maximum efficiency. Often weight, size or cost may be an overriding issue. Nevertheless, given an operating condition for the thermoelectric converter, defined by the hot and cold side temperatures and the heat flux, the converter should operate at maximum efficiency. Finding the optimum efficiency and length for any operating condition gives the following functions

$$\eta = \eta_{\max}(T_h, T_c)$$
$$l = l(T_h, T_c, Q_{total}/A_{total})$$

Which can be incorporated into the system model to find the optimal system operation condition.

For example, often in a thermoelectric generator the power/mass is the primary concern. In this case, the power/mass can be increased by reducing the mass of the heat exchangers at the cost of reducing the temperature difference which lowers the efficiency. By knowing how the optimum efficiency and length vary with input temperature and heat flux, the exact system solution is found without requiring the systems analysis to be capable of thermoelectric calculations. Once the system trades are complete, the final configuration of the thermoelectric generator can be determined. Given the total power and voltage required, the size and number of couples can be established. The minimum number of couples is determined by the voltage requirement. The voltage produced V_{system} is the number of couples connected in series N_{series} times the couple voltage V_{couple} (equation 14).

$$V_{system} = V_{couple}N_{series} \tag{23}$$

Often redundancy is desired by including additional parallel circuits $N_{parallel}$.

$$N_{system} = N_{series}N_{parallel} \tag{24}$$

With the thermoelectric length now fixed, the total power produced defines the total cross sectional area. With the total area, length (from equation 20) and number of couples N_{system}, the couple geometry can now be determined.

$$A_{couple} = \frac{P}{\frac{P}{A_{total}} N_{system}} \tag{25}$$

Non Optimal Operating conditions

Once the optimal configuration is established, the performance at non-optimal conditions, such as the full I-V curve can be calculated. In general, the heat flow, the temperatures, and the current can all vary from the optimal but the geometry remains fixed. The heat flow and temperatures will change in a correlated way determined by the thermal impedance of the components external to the thermoelectric converter, just as the electrical current will change due to a change in the external electrical impedance.

Given the electrical current in the generator and two out of three of the heat flux, hot and cold side temperatures (or equivalent relationships), the relative current density u, and therefore the generator characteristics can be determined.

For example, if the hot and cold side temperatures are known (*e.g.* remain constant for low external thermal impedance) the relative current density $u(T)$ of each element can be calculated (and estimated with $\approx$) from

$$\int_{T_c}^{T_h} u\kappa dT = I\frac{l}{A} \approx \bar{u}\,\bar{\kappa}\Delta T \tag{26}$$

If the effective external thermal impedance is high, an *IV* curve can be calculated assuming the heat supplied remains constant (and the hot or cold side temperature or a relationship is given). In this case, the three unknowns (the unknown temperature, and an initial value for u_n and u_p) are solved from three equations: two of the form (26), for *n*-type and *p*-type, and the heat flow (at $T = T_{hot}$ if the hot side heat flow is known) from (6) for the couple:

$$Q = I(\Phi_p - \Phi_n) = I\left(\alpha_p T + \frac{1}{u_p} - \alpha_n T - \frac{1}{u_n}\right) \tag{27}$$

For low current operation, the Peltier cooling at the hot end of the thermoelectric will decrease, requiring an increase in the hot side temperature and the interface temperatures. Such high temperature operation may advance the degradation of the thermoelectric materials. If such degradation is detrimental to system performance, lower optimal operation temperatures should be selected.

Because the geometry of the elements does not change (in particular the length and area of each segment) the interface temperatures between the segments will change from their optimal values. The interface temperatures can be found by finding the interface temperatures that keep the lengths of each segment constant (Equation (27)). Even for low external thermal impedance, where the hot and cold side temperatures remain constant, the interface temperatures between the segments will change somewhat with varying electrical current.

Non Ideal Thermoelectric Converters

Thermal and electrical contact resistances are unavoidable in thermoelectric converters. In "ideal" systems [7] there are no contact resistances but in real systems they must be considered. The non-idealities can be considered part of the system design, as long as the temperatures and heat flux into the thermoelectric elements are well defined.

Conclusions

In this paper the design of a segmented thermoelectric generator is outlined. First, high zT materials with similar compatibility factors are selected. Then the efficiency is optimized with respect to the relative current density and the interface temperatures between the segments. This is accomplished for all hot and cold side temperatures, which along with the length of the thermoelectric elements (derived from the desired heat flux density) is used in the system analysis to find the overall optimum operating conditions. In this way, the desired system configuration, whether it is maximum efficiency or power per weight is defined.

For calculations, the thermoelectric potential is used to compute the exact result for materials with temperature dependent thermoelectric properties. This calculation does not assume constant or averaged thermoelectric properties as is often done for analytic results. In the calculations, the relative current density is the intensive independent variable of prime concern.

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References

[1] G. J. Snyder and T. Ursell, "Thermoelectric Efficiency and Compatibility" *Phys. Rev. Lett.*, in press (2003).

[2] B. Sherman, R. R. Heikes, and R. W. Ure, "Calculation of Efficiency of Thermoelectric Devices" *J. Appl. Phys.* **31**, 1 (1960).

[3] T. S. Ursell and G. J. Snyder, "Compatibility of Segmented Thermoelectric Generators" in *Twenty-first International Conference on Thermoelectrics. Proceedings, ICT'02* (IEEE, Long Beach, California, USA, 2002), p. 412.

[4] A. E. Kaliazin, V. L. Kuznetsov, and D. M. Rowe, "Rigorous Calculations Related to Functionally Graded and Segmented Thermoelements" in *Proceedings ICT2001. 20 International Conference on Thermoelectrics*, 2001), p. 286.

[5] R. W. Cohen and B. Abeles, "Efficiency Calculations of Thermoelectric Generators with Temperature Varying Parameters" *J. Appl. Phys.* **34**, 1687 (1963).

[6] B. Sherman, R. R. Heikes, and R. W. Ure, in *Thermoelectric Materials and Devices*, edited by I. B. Cadoff and E. Miller (Reinhold, New York, 1960), p. 199.

[7] G. Min and D. M. Rowe, in *Thermoelectric Handbook*, edited by D. M. Rowe (CRC, Boca Raton, 1995), p. 479.

[8] R. R. Heikes and R. W. Ure, *Thermoelectricity: Science and Engineering* (Interscience, New York, 1961).

[9] M. H. Cobble, in *Thermoelectric Handbook*, edited by D. M. Rowe (CRC, Boca Raton, 1995), p. 489.

[10] D. L. Kerr, in *Thermoelectric Materials and Devices*, edited by I. B. Cadoff and E. Miller (Reinhold, New York, 1960), p. 227.