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Uncertainty and sensitivity of the maximum power in thermoelectric generation with temperature-dependent material properties: An analytic polynomial chaos approach

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ABSTRACT

In this article, the technique of polynomial chaos expansion is combined with an analytic model of thermoelectric power generation to quantify the uncertainty and sensitivity in the performance indices of thermoelectric generation, due to the uncertainty in the temperature-dependent material properties. The Seebeck coefficient, electrical resistivity, and thermal conductivity are given in the form of second-order polynomials in temperature, whose coefficients follow normal probability distributions. The model is used to analytically estimate the mean and standard deviation of the output parameters and to generate cheap ensembles for constructing the probability density functions. The uncertainty in the maximum power density and other associated properties is quantified, and the results are compared to those obtained from direct Monte Carlo simulations. The first-order and total sensitivity indices are also presented. The model can estimate the uncertainty accurately, although the standard deviation in the current density at the maximum power condition has shown some deviation from that of the Monte Carlo simulation. Even the first-order polynomial chaos expansion performs well in our cases, because thermoelectric effects can be essentially considered as a first-order perturbation in thermoelectric generation due to its low energy conversion efficiency.

1. Introduction

Thermoelectric generators (TEGs) made with thermoelectric (TE) materials are solid-state devices that operate without any moving parts and hence can be useful as compact waste heat recovery systems in vehicles or for electricity generation in isolated or extreme environments [1,2]. TEGs are also considered as part of hybrid generation systems when combined with solar cells or fuel cells [3–5]. Typically, the maximum conversion efficiency of thermoelectric power generation (η_{MAX}) is expressed in terms of the temperature of each heat reservoir and the thermoelectric figure of merit $ZT = (\alpha^2 T)/(\rho k)$, where α is the Seebeck coefficient, ρ is the electrical resistivity, k is the thermal conductivity, and T is the temperature [6]. As ZT is one of the most important control parameters for the efficiency of thermoelectric energy conversion, significant efforts have been exerted on creating materials with high ZT values. Approaches to improve the performance of materials include construction of superlattices [7], nanowires [8], nanostructured grains [9] or hierarchical spatial structures [10], insertion of multiple guest elements [11], careful modification of compositions [12], and improvement of phase purity [13]. There also have been research efforts for improving the system performance of TEGs by adjusting leg geometry and module shapes [14–16], enhancing external heat transfer processes [17,18], and changing the morphology of the thermoelectric elements [19,20].

Compared to the huge attention given to the development of advanced TE materials and systems by the research community, relatively little attention has been placed on systematic quantification of uncertainty and sensitivity of the performance indices of TE generation. Considering enormous potential uncertainty in the intriguingly subtle tuning process of TE materials and the enormously complex manufacturing process of TE systems, this is a rather surprising situation. Only a few previous studies have addressed the sensitivity of TE cooling systems [21,22]. A detailed sensitivity analysis using a numerical model of TE cooling systems was performed in [21]. Another study [23] performed a sensitivity analysis of TE generation systems, but the uncertainty due to material aspects was not considered in details; the study mostly focused on the geometric features of the generation systems.

In this article, the technique of polynomial chaos expansion (PCE) [24–26] is analytically applied to quantify the uncertainties in the performance indices of TE generation due to the uncertain material properties. The material properties relevant to ZT, i.e., Seebeck

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Nomenclature

A_0, A_1, A_2, B_0, B_1, B_2, C_0, C_1, and C_2	random coefficients in the polynomial fits of material properties
j	current density
j_{MP}	current density at the maximum power condition
K_1 and K_2	parameters in the expression of q_h''
k	thermal conductivity
L	length of the thermoelectric element
M_1, M_2, M_3, M_4, M_5, and M_6	parameters in the expression of q_h''
P	probability density function (PDF)
q_c''	heat flux at the end on the cold side
q_h''	heat flux at the end on the hot side
S_i and S_{ij}	first-order sensitivity indices, Eqs. (25) and (26)
S_{Ti}	total sensitivity indices, Eq. (27)
T	temperature
T_c	cold side temperature
T_h	hot side temperature
T_m	$T_m = (T_h + T_c)/2$
ΔT	$\Delta T = T_h - T_c$
V_i and V_{ij}	defined in Eqs. (28) and (29)
w''	power density
w''_{MP}	maximum power density
X_n	a generic variable representing one of A_0, A_1, A_2, B_0, B_1, B_2, C_0, C_1, and C_2
$\overline{X_n}$	mean of X_n
ZT	figure of merit, $ZT = (\alpha^2 T)/(\rho k)$
α	Seebeck coefficient
β_a^m	the mth PCE coefficient of the variable a
η	conversion efficiency
ξ_{Xn}	standard normal random variable associated to X_n
ρ	electric resistivity
σ_{Xn}	standard deviation of X_n
Ψ^m	the mth Hermite polynomial

coefficient (α), electrical resistivity (ρ), and thermal conductivity (k), are given in the form of second-order polynomials in temperature, as in previous studies [21,27,28]. The coefficients of the polynomials bear uncertainties following certain probability distributions. The performance indices are estimated based on an approximate analytic model of TE generation [29], which is modified in order to incorporate the PCE. The model enables us to analytically construct the PCE of the relevant performance indices, avoiding the curse of dimensionality during the evaluation of the coefficients in the PCE. The uncertainties in the maximum power density and the associated current density are quantified, and the results are compared to those obtained from direct Monte Carlo (MC) simulations.

The paper is organized as follows. In Section 2, the PCE of the performance indices for TE generation is constructed analytically. In Section 3, we apply the PCE model to a half-Heusler alloy [30]. Comparison of the results from the PCE model against the direct MC simulations is provided to demonstrate the accuracy of the PCE model. In Section 4, conclusions are drawn by summarizing the results.

2. Polynomial chaos expansion applied to thermoelectric power generation

The PCE model of TE power generation developed here is largely based on the model developed in [29]. Let us consider a single thermoelectric element as shown in Fig. 1, whose length is L, placed between two thermal reservoirs. T_h and T_c represent the temperature of the hot reservoir and that of the cold reservoir, respectively. q_h'' is the heat flux from the hot reservoir, and q_c'' is that to the cold reservoir. The power density (w'') is equal to $q_h'' - q_c''$. j is the current density. The material properties are given in the form of second-order polynomials [21,27,28]:

$$\alpha = A_0(1 + A_1(T - T_m) + A_2(T - T_m)^2), \tag{1}$$

$$\rho = B_0(1 + B_1(T - T_m) + B_2(T - T_m)^2), \tag{2}$$

and

$$k = C_0(1 + C_1(T - T_m) + C_2(T - T_m)^2), \tag{3}$$

where each X_n coefficient ($X = A$, B, or C, and $n = 0$, 1, or 2) is a random variable, independent of one another. T represents temperature, and T_m is $(T_h + T_c)/2$.

In this note, we consider normal distributions; hence, each X_n coefficient acquires the following form:

$$X_n = \overline{X_n}(1 + \sigma_{Xn}\xi_{Xn}), \tag{4}$$

where $\xi_{Xn} \sim \mathcal{N}(0,1)$. Normal distributions are assumed for simplicity, but the approach can be used for other probability distributions as well. $\overline{X_n}$ and σ_{Xn} represent the mean and standard deviation of each X_n variable, respectively.

Making several approximations including the major assumption that the material properties could be evaluated from a linear temperature profile between the hot end and the cold end, analytic closed-form expressions for several important performance indices were obtained in [29]. The entire procedure of such analysis is not reproduced here. Instead, we simply demonstrate how the PCE method [24–26] is incorporated into the analytic model.

We begin with the power density w''. In [29], it was demonstrated that the power density could be calculated:

$$w'' = j\left(A_0\Delta T\left(1 + \frac{A_2\Delta T^2}{12}\right) - jB_0L\left(1 + \frac{B_2\Delta T^2}{12}\right)\right). \tag{5}$$

ΔT is $T_h - T_c$. With the expression of Eq. (4), w'' becomes

$$w'' = j\left\{\overline{A_0}(1 + \sigma_{A0}\xi_{A0})\Delta T\left(1 + \frac{\overline{A_2}(1 + \sigma_{A2}\xi_{A2})\Delta T^2}{12}\right)\right.$$
$$\left. - j\overline{B_0}(1 + \sigma_{B0}\xi_{B0})L\left(1 + \frac{\overline{B_2}(1 + \sigma_{B2}\xi_{B2})\Delta T^2}{12}\right)\right\}. \tag{6}$$

From Eq. (5), one can easily deduce that the maximum power density occurs when $j = j_{MP}$, where

$$j_{MP} = \frac{A_0\Delta T}{2B_0L} \times \frac{12 + A_2\Delta T^2}{12 + B_2\Delta T^2}. \tag{7}$$

Again, with Eq. (4), it becomes

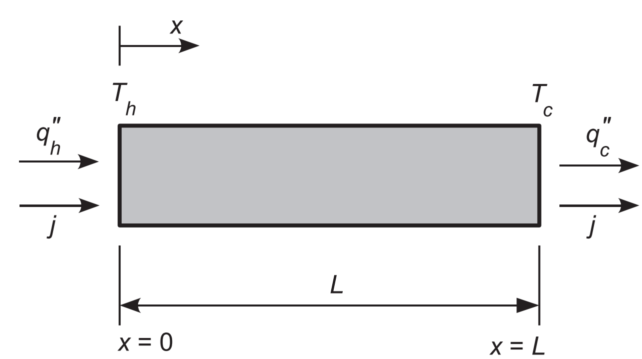

Fig. 1. Schematic illustration of a single thermoelectric element. The hot and cold ends maintain T_h and T_c, respectively.