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Notes on Computational Methodology and Tools of Thermoelectric Energy Systems

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Abstract

The SPICE model allows the concurrent simulation of thermoelectric devices and application electric sub-models. It is an important step to implement the thermoelectric modeling at the system level. In this paper, temperature dependent material properties in the SPICE model, temperature and heat flow obtained by the code ANSYS Multiphysics and SPICE (Simulation Program with Integrated Circuit Emphasis), as well as some notes on the 3-D extension of the SPICE model are introduced.

Keywords: Thermoelectric Energy Systems, Temperature polynomial functions

1. Introduction

The simple analytical one-dimensional (1-D) model of thermoelectric generators (TEG) and thermoelectric coolers, which is very often referred in the literature, can be derived both from the classical heat transfer theory [1, 2] and from irreversible thermodynamics [3]. With an emphasis on a clear formulation of boundary conditions, we have compared the derivations of the simplified 1-D analytical model based upon the governing equations of both approaches, and arrived to a unified result for the analytical model of thermoelectric devices under both theoretical frameworks of irreversible thermodynamics and heat transfer, respectively [4]. In other previous studies [5, 6] we have introduced the numerical electro-thermal analogy using the finite-difference method (FDM) into the description of the 1-D TEG differential equation, and investigated the heat transfer problem of TEG by the circuit simulator SPICE.

Our numerical TEG model of the electro-thermal analogy is based on the conventional heat transfer formulation. Yet there have been other irreversible thermodynamics based works on numerical modelling of TEG by finite element method (FEM) [7] and finite volume method (FVM) [8]. A preliminary comparison of two different kinds of computational tools shows that the numerical approximation methods based on irreversible thermodynamics in principle do not suffer more essentially theoretical drawbacks than the conventional heat transfer methods. Both the ANSYS model and the SPICE model have the ability of convenient interaction between thermal and electrical circuits, calculating temperature dependency of materials properties, and others. However, since the heat transfer numerical formulation by SPICE has more customized governing equations and is more flexible, its results might be easier to analyze and to truly understand [4].

The intention of this presentation is to investigate the details of the comparison of simulation results from ANSYS and SPICE. The comparison is based on a same set of thermoelectric material temperature data. The details in fitting the temperature dependency of these material properties by polynomial functions will be presented, serving as an appendix to the work published elsewhere [9]. The temperature and heat flow profiles obtained by ANSYS and SPICE will be compared and analysed. Some notes on the 3-D extension of the SPICE model, i.e., grid generation, meshing, and node connection methodology, are furnished.

2. Temperature polynomial functions for thermoelectric material properties

The example considered is the thermoelectric generator described in [7]. The temperature dependent material properties used in the simulation are the n- and p-type bismuth telluride alloys brought alone by ANSYS. Temperature data points range is from $300K$ to $625K$ with a span of $25K$. The three principal properties of the p-type and n-type materials, i.e., the Seebeck coefficient $\alpha_{p,n}$, the electrical resistivity $\rho_{p,n}$, and the thermal conductivity $k_{p,n}$, are measured at each temperature data point. ANSYS defines the material properties in terms of a fourth order polynomial as a function of temperature. If the constants C_0 - C_4 are input, the polynomial

$$Property = C_0 + C_1 T + C_2 T^2 + C_3 T^3 + C_4 T^4 \tag{1}$$

is evaluated at discrete temperature points with linear interpolation between points and a constant-valued extrapolation beyond the extreme points [10]. For the SPICE model, two, three, or four order polynomial functions in MATLAB fit the temperature dependency of these material properties. Tables 1 and 2 show the constants C_0 - C_4 of the polynomial functions. Figures 1- 4 show the values of material properties at temperature points. The temperature dependency is approximated by polynomial functions.

Table 1: Constants C_0 - C_4 of the polynomial functions of the temperature dependent material properties used for the SPICE model: n-type material

	α_n	ρ_n	k_n
C_0	1.0e-4 * 0.51499314285715	1.0e-4 * 0.54262451822436	-1.27330643491471
C_1	1.0e-4 * -0.01040748901099	1.0e-4 * -0.00341277909918	0.01645469397959
C_2	1.0e-4 * 0.00001122527473	1.0e-4 * 0.00000834046941	-0.00003406693354
C_3	0	1.0e-4 * -0.00000000610010	0.0000000218467
C_4	0	0	0

Table 2: Continued with p-type material

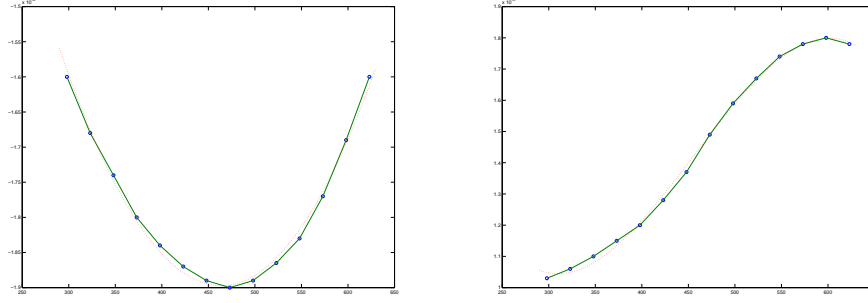|	α_p	ρ_p	k_p
C_0	0.00275280431679	1.0e-4 * 0.39369469841970	13.04091244704822
C_1	-0.00002622419289	1.0e-4 * -0.0031132439573	-0.13921081730663
C_2	0.00000009738114	1.0e-4 * 0.00000950850068	0.00058137561961
C_3	-0.0000000015387	1.0e-4 * -0.00000000806198	-0.00000103243586
C_4	0.000000000000086878	0	0.00000000066175

Figure 1: Temperature dependent Seebeck coefficient α_n (left) and temperature dependent electrical resistivity ρ_n (right) of the n-type bismuth telluride alloy and their polynomial approximations.

3. A comparative study of computational tools of thermoelectricity

As shown in [9], numerical results from SPICE match almost exactly those from ANSYS, and the SPICE model is an equivalent thermal simulator to ANSYS in 1-D thermoelectric simulation. Thus the temperature profiles obtained by ANSYS and SPICE should be identical. It is of our main interest herein to compare the heat flow from the simulation results of a TEG. In [4] whence the ANSYS element solution is shown, it is found out that in both n-type and p-type legs the thermal flux monotonically decreases from the hot junction to the cold junction. One thing this means is that the Thomson heat and the conduction flow are inextricable in the total heat flow as one form of the irreversible thermodynamics flux. But the SPICE model proffers a new option to study the effects of the Thomson heat. For the TEG instance brought alone by ANSYS, the Thomson heat caused by the temperature dependent Seebeck coefficient as well as the Joule heat can be calculated by SPICE, listed in Table 3. In a recent paper it is argued that the magnitudes of the Peltier, Joule, and Thomson heats are commensurable [11]. With the SPICE thermoelectric model and Table 3 in hands, such postulations can be judged easily.
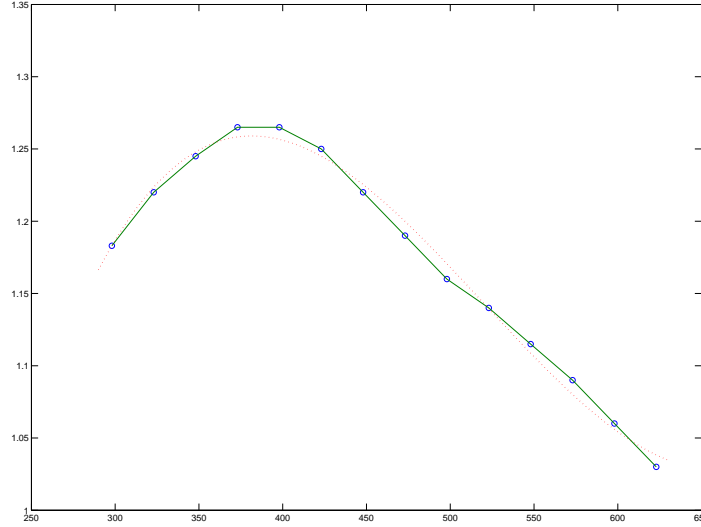
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Figure 2: Temperature dependent thermal conductivity k_n of the n-type bismuth telluride alloy and its polynomial approximation.

4. Implementation of convection/radiation source terms and 3-D thermal resistor network by SPICE

Since certain TEG parameters could not be accurately predicted using the 1-D TEG thermal model, the importance of 3-D thermal analysis is fairly verified. Obviously the main results of a 3-D thermal analysis are supposed to be 3-D. Temperature distribution, for instance, should be expressed as $T(x, y, z)$ and used in the electric analysis to get the total Seebeck voltage generated by the TEG as we have stressed before. Bearing the non-ohm current-voltage relation in both legs of the device in mind, the electric field in a TEG, including electric current and potential, is 3-D, i.e., $I(x, y, z)$ and $V(x, y, z)$. In addition, although the 1-D analysis is fast and easy to run, its lack of details on lateral distributions of electric potential and current makes impossible to obtain the effective electrical resistance. Therefore, the 3-D electric field analysis of a TEG, by which the main results can be obtained, should be as important as the 3-D thermal field analysis. The load current-load voltage relation, however, still fulfills the general Ohm law, and the generic analytical equations about performance on the load are still applicable. There is no need to consider the power output in a 3-D way. The general multidimensional multi-physics numerical scheme for TEG can be upgraded from the one shown therein [9] to a new flow chart form.
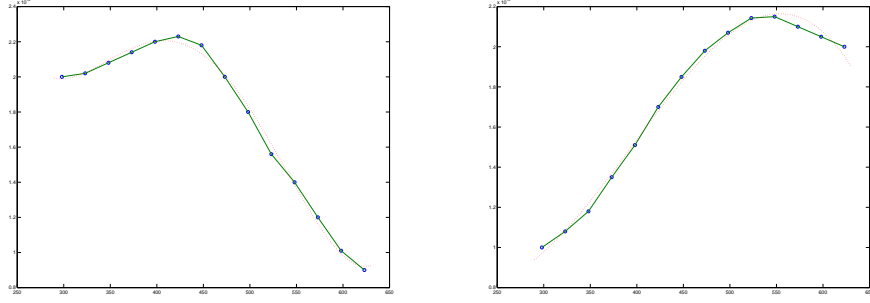
Figure 3: Temperature dependent Seebeck coefficient α_p (left) and temperature dependent electrical resistivity ρ_p (right) of the p-type bismuth telluride alloy and their polynomial approximations.

Table 3: SPICE simulation results. The Thomson and Joule heat along the p-and n-type legs for TEG with temperature dependent material properties [7]

cell position	p-type	p-type	n-type	n-type
	Thomson heat	Joule heat	Thomson heat	Joule heat
1	$355.8mW$	$77.5mW$	$122.5mW$	$79.69mW$
2	$419.0mW$	$76.91mW$	$56.52mW$	$74.41mW$
3	$221.6mW$	$70.13mW$	$7.868mW$	$66.63mW$
4	$42.73mW$	$60.54mW$	$29.14mW$	$58.34mW$
5	$60.4mW$	$50.05mW$	$59.02mW$	$51.21mW$
6	$61.89mW$	$39.71mW$	$85.67mW$	$47.06mW$

In [12], SPICE implementation of convection/radiation source terms and 3-D thermal resistor network of TEG are presented. For simplicity, the current source model in a series form was used as the control volume in the illustrations of convection and radiation terms on the surface elements, 2-D grid of the middle plane, and the connection of planes of the cubic grid [12]. It is noted that another scheme with equivalent current sources connected in parallel with the resistor should be adopted instead in the actual network to include the temperature
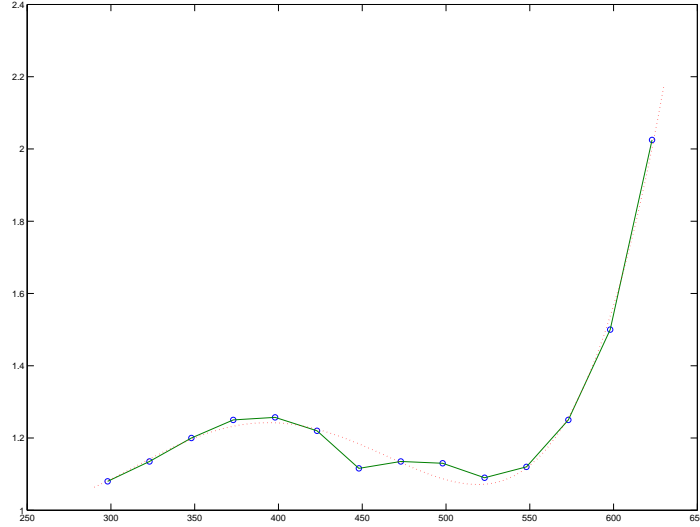
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Figure 4: Temperature dependent thermal conductivity k_p of the p-type bismuth telluride alloy and its polynomial approximation.

dependent thermal conductivity. The difference between the two schemes is clearly explained in [9].

5. Concluding remarks

In order to identify the impact of incorporating thermoelectric devices into existing energy systems, as well as to design a new generation of applications to include these devices, the interaction of application thermal and electric sub-models with the thermoelectric device model should be included in the simulation. The SPICE model of thermoelectric devices discussed in this paper can be simulated together with application electric sub-model as a system level simulation. The further challenge of modeling thermoelectricity at the system level therefore consists of the development of application thermal sub-models, known as other pertinent engineering tasks. In the development of such models we mainly address the issue of how to computationally simulate the fluid - heat transfer coupled multi-physics effects, where the temperature gradients across the top and bottom surfaces of the devices and those across the contact surfaces of the heat and cold sources should depend upon each other. Various application examples of energy system simulation based on CFD technology are numerically presented for analysis. The practical application scenarios and the

interaction between sub-models are precisely described by using the third kind of thermal boundary conditions instead of the first and the second.

On the other hand, to overcome the drawback of the presented FDM and Newton-Raphson scheme, i.e. the visualization of the simulation results, we try to integrate those 3-D datasets from the multi fields into a common Visualization Engineering Suite framework. A complete analysis of irreversible transfer processes of thermoelectricity is realized as a physics-based virtual system by integrating computational results from the multi-fields into a common Visualization Engineering Suite framework. The immersible visual environment allows a robust optimization and design tool for thermoelectric devices described by the heat transfer numerical model, and facilitates the access to the analysis of performance of thermoelectric devices in an intuitive and interactive manner. These are reserved for later publication.

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