Heat Transfer in Thermoelectricity: Modelling, Optimization and Design

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Abstract: - Two methods are used to solve the heat transfer equation in a thermoelectric leg: analytical and numerical. Simulations are performed with the software FlexPde based on finite element method. The influence of the Thomson effect and also the non linearity due to the thermodependence of the thermophysical parameters are investigated. Results in terms of temperature and fluxes are presented. Then the case of a segmented leg (sandwiched structure) used in Radioisotope Thermoelectric Generators is studied through the compatibility factors and reduced efficiency.

Key-Words: - Thermoelement, heat transfer, modelling, simulations, efficiency, design, segmentation, RTGs

1 Introduction

When a temperature difference exists, a potential for power production ensues: it is the principle of thermoelectricity, it could provide an unconventional energy source for a wide range of applications even if the efficiency [1] of the thermoelements is rather low. As a consequence, there is an increasing use of thermoelectric devices in many fields such as aerospace [2-4], automotive [5] and also envisaged for recovering heat from nuclear waste during storage [6]. On the other hand, the coupled effects involved in such systems usually lead to complex modelling. In order to predict the performances of the device, several methods could be used: experimental, numerical and semi-analytical. For the experimental ones, the device must already exist whereas numerical and semi-analytical methods could provide more or less realistic predictions. Let investigate the modelling of a thermoelectric leg in order to estimate for instance its coefficient of performance or to design segmented thermoelements applied to Radioisotope Thermoelectric Generators.

2 Heat transfer in a thermoelectric leg

In this part, a thermal modelling of a thermoelectric leg is presented in order to better understand the underlying physical phenomena and the contribution of the different effects. The aim is to determine the expressions of the temperature within the thermoelement and also the heat fluxes. Indeed these two quantities are needed to determine the performance of the device by calculating the efficiency of the element or for instance by evaluating the COP. The Joule contribution is taken into account (introducing a source term in the heat transfer equation) and the effect due to the Thomson coefficient is investigated.

2.1 Problem formulation

Consider a single thermoelectric leg of length l and cross-sectional area A. An electrical current $I=JA$ enters uniformly into the element. The one-dimensional energy balance [7-9] that describes the thermal behaviour of the leg is the following partial differential equation

$$\rho c_p \frac{\partial T(x,t)}{\partial t} = \lambda \frac{\partial^2 T(x,t)}{\partial x^2} + \frac{J^2}{\sigma} - \tau J \frac{\partial T(x,t)}{\partial x} \qquad (1)$$

The temperature is a function of the spatial variable x and the time t. The relevant material properties are the density ρ, the heat capacity c_p, the thermal conductivity λ, the electrical conductivity σ.

In the steady-state case, the classical boundary conditions are the following ones: the hot side of the leg is at absolute temperature T_H and the cold side at temperature T_C.

2.2 Problem solution

To solve the heat transfer equation (1), two methods are considered:

- an analytical method which assumes that the thermophysical properties are constant on the temperature range considered
- a numerical method which uses the finite element method and takes the non linear thermodependence of the thermophysical parameters into account.

2.2.1 Analytical method

The equation (1) becomes a classical ordinary differential equation [10]. If the Thomson effect is taken into account, the temperature within the leg is then given by the analytical expression:

$$T(x) = T_C + \frac{J}{\sigma\tau} x + \frac{T_H - T_C - \dfrac{J}{\sigma\tau} L}{\left(1 - exp\left(\dfrac{\tau J}{\lambda} L\right)\right)} \left(1 - exp\left(\frac{\tau J}{\lambda} x\right)\right) \qquad (2)$$

If the Thomson effect is neglected, the expression of the temperature contains no exponential but quadratic terms:

$$T(x) = T_C + \left(\frac{T_H - T_C}{L} + \frac{J^2 L}{2\sigma\lambda} \right) x - \frac{J^2}{2\sigma\lambda} x^2 \quad (3)$$

2.2.2 Numerical simulations with FlexPde

Numerical simulations have been performed with FlexPde. This software solves the partial differential equations with the finite element method and allows to take into account the non linearity due to the thermodependence of the coefficients appearing along the partial differential equation. The mesh chosen to ensure a good convergence of the simulations contains 2365 nodes and 1138 cells and the error is about 10^{-7}. The data used for the simulations are summarized in the table below.

Table 1: Data used for the simulations

Temperature cold side ($x=0$)	$T_C = 270K$
Temperature hot side ($x=L$)	$T_H = 300K$
Length	$L = 1.4\ 10^{-3} m$
Constant section	$A = 1.4\ 10^{-6}\ m^2$
Thermal conductivity	$\lambda = 1.701\ Wm^{-1}K^{-1}$
$\lambda(T) = (62605 - 277.7\ T + 0.4131\ T^2)\ 10^{-4}\ Wm^{-1}K^{-1}$	
Electrical resistivity	$\rho = 1.027\ 10^{-5}\ \Omega m$
$\rho(T) = (5112 + 163.4\ T + 0.6279\ T^2)\ 10^{-10}\ \Omega m$	
Seebeck coefficient	$\alpha = 2.07\ 10^{-4}\ V/K$
$\alpha(T) = (22224 + 930.6\ T - 0.9905\ T^2)\ 10^{-9}\ V/K$	
Thomson coefficient	$\tau = 1.04\ 10^{-4}\ V/K$
$\tau(T) = (930.6 - 0.9905\ T^2)\ 10^{-9}\ T\ V/K$	

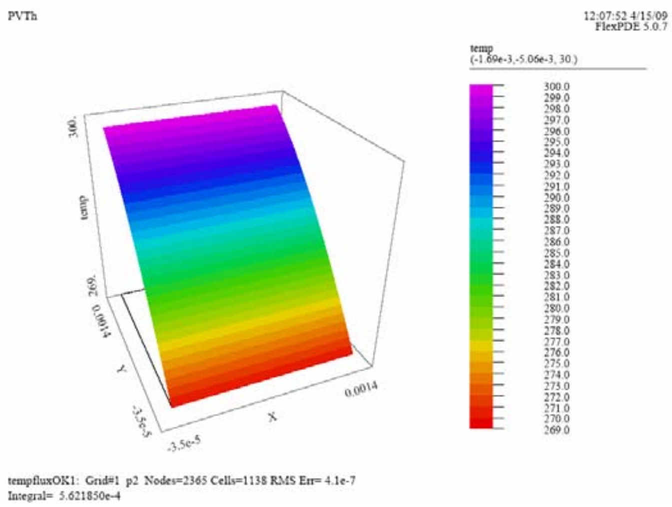

Figure 2 : Temperature along the leg (simulations performed with FlexPde, thermodependence of the coefficients)

The temperature field in the thermoelectric leg obtained with the software FlexPde is plotted in the figure 2. The major advantage of the numerical simulations is the ability to take the variations of the coefficients with the temperature into account. The values chosen for the thermophysical parameters correspond to a real case of a thermoelectric leg with thermophysical properties measured and measurements fitted by curves.

2.3 Temperatures

In this section, several results concerning the temperature are presented. First of all, the results obtained with the analytical model and the numerical model based on finite element method are compared in the Figure 3. One notes a good agreement between the two curves.

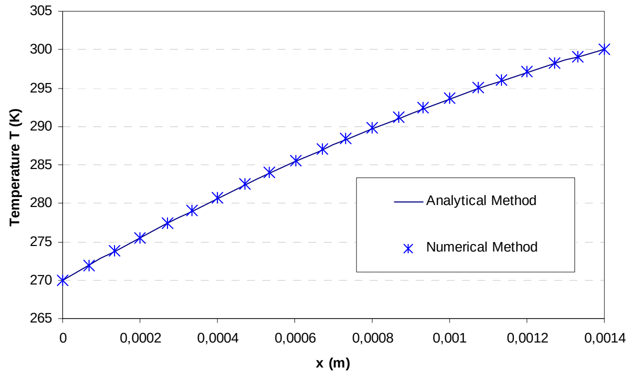

Figure 3 : Comparison of the temperature field obtained with the analytical model and the numerical model

Then the influence of the Thomson effect is investigated (because in many studies it is often neglected [10, 11]). The temperature is plotted in the Figure 4 without Thomson effect and also for a Thomson coefficient $\tau = 1.04e^{-4}\ VK^{-1}$. The maximum difference could achieve 3.4 K and is obtained at the middle of the leg. For a positive value of τ, the Thomson effect has a "cooling" effect.

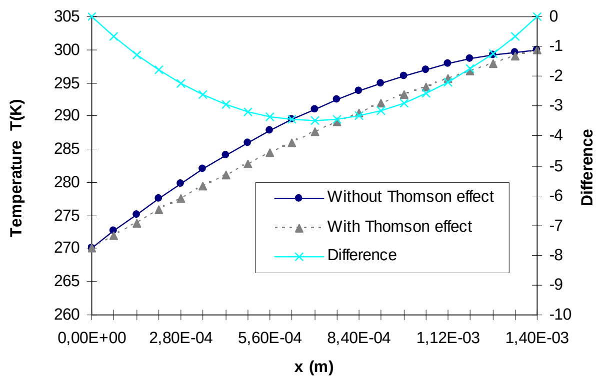

Figure 4 : Comparison of the temperature field obtained with or without the Thomson effect

2.4 Fluxes and entropy generation

It is although interesting to have the expression of the flux going through the thermoelement in order to have a complete modelling of the heat transfer within the leg.

The flux is a linear combination of the temperature and the derivative of the temperature. Its expression φ and also the expressions of the entropy flux density *Js* and of the entropy generated *Sgen* are summarized and plotted in the figures below.

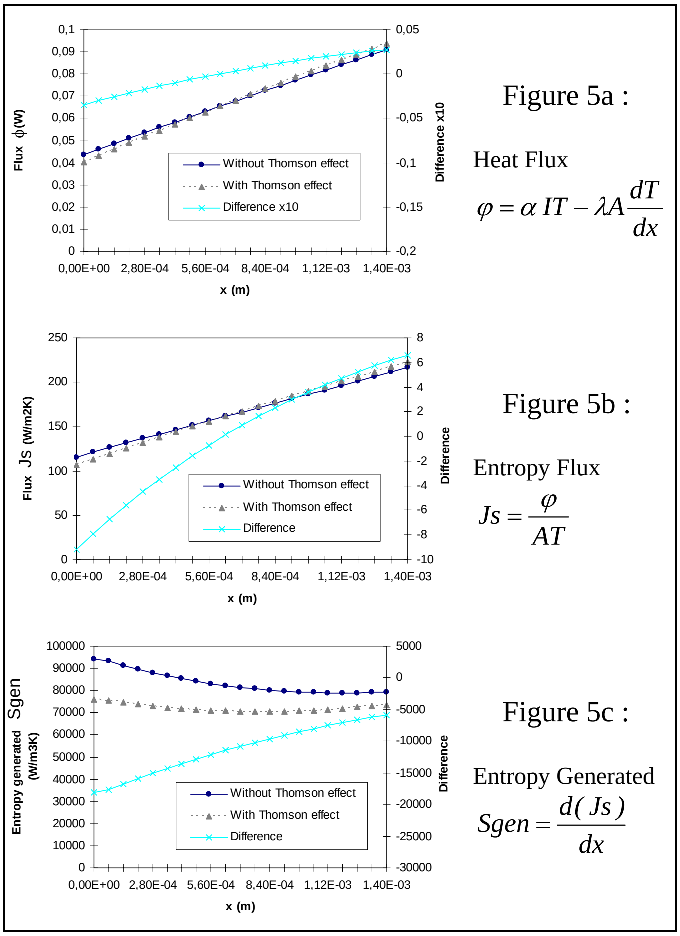

Figure 5: Fluxes and Entropy generated

Once the temperature and the fluxes determined, it is then possible to evaluate the coefficient of performance of the thermoelectric device. It is also interesting to have an idea of the entropy generated in order to design a thermoelectric device with minimizing this creation.

In this second part the heat transfer in a simple thermoelectric leg (only constituted by one material) has been investigated. In the following part, a more complex thermoelectric leg (composed by several materials) will be envisaged for space applications.

3 Design applied to RTGs

In this third part, the design of a thermoelement for instance applied to Radioisotope Thermoelectric Generators (RTGs) [2] is investigated.

3.1 Background and segmentation

As no single thermoelectric material presents high figure of merit over a wide temperature range, it is therefore necessary to use different materials and to segment them together in order to have a sandwiched structure: in this way, materials are operating in their most efficient temperature range [12, 13].

Even if the thermoelectric figure of merit is an intensive material property of prime importance, it is not the only one: indeed the expression of the reduced efficiency involves another parameter called the compatibility factor [14], which must be considered and controlled to determine the relevance of segmentation.

Not only the reduced efficiency but also the compatibility factors are then plotted for different n-type and p-type elements such as skutterudite as function of the temperature. Thanks to these considerations, the design of the segmented thermoelectric device is investigated in order to optimize the efficiency and once the materials chosen, to determine the best operating conditions and especially the relative current density which is the ratio of the electric current density to the heat flux by conduction.

3.2 Principle of the method on a test case

3.2.1 Some equations

Before considering the compatibility factor and the reduced efficiency, some equations have to be remembered. (for more details see references [4;14]) such as for instance the relative current density which is the ratio of the electric current density to the heat flux by conduction:

$$u = J/\lambda\nabla T \tag{4}$$

The variation of u is governed by the heat equation and then satisfies the following differential equation:

$$\frac{d(1/u)}{dT} = -\frac{1}{u^2}\frac{du}{dT} = -T\frac{d\alpha}{dT} - u\,\rho\,\lambda \tag{5}$$

where the Seebeck coefficient α, the resistivity ρ and the thermal conductivity λ can be functions of temperature.

The reduced efficiency is defined as the power produced divided by the power supplied to the system:

$$\eta_r = \frac{E \cdot J}{-\nabla T \cdot J_S} = \frac{E \cdot J}{-\dfrac{\nabla T}{T}\cdot q} = \frac{\alpha\, J \cdot \nabla T - \rho\, J^2}{\dfrac{\lambda}{T}(\nabla T)^2 + \alpha\, J \cdot \nabla T} \tag{6}$$

It could be expressed as a function of u and of the thermoelectric figure-of-merit z:

$$\eta_r(u) = \frac{u\dfrac{\alpha}{z}\left(1 - u\dfrac{\alpha}{z}\right)}{u\dfrac{\alpha}{z} + \dfrac{1}{zT}} = \frac{1 - u\dfrac{\alpha}{z}}{1 + \dfrac{1}{u\alpha T}} \tag{7}$$

The aim is to optimize this quantity. The value of the relative current density which gives the largest reduced efficiency is noted s and called the thermoelectric compatibility factor [14]:

$$s = \frac{\sqrt{1+zT}-1}{\alpha T} \tag{8}$$

The compatibility factor depends on the temperature, on the Seebeck coefficient and on the figure of merit which involves the Seebeck coefficient but also the thermal conductivity and the electrical conductivity.

If the compatibility factors of materials which must be segmented together differ by a factor 2 or more, a value of the relative current density can not be suitable for both materials and it is obvious that the working point could not be optimum for the both together. In that case, the segmentation is not useful and does not allow to increase the efficiency.

Then the two quantities on which the attention is focused now are the thermoelectric compatibility factor and its evolution versus temperature and the reduced efficiency and its evolution as a function of the relative current density.

3.2.2 Compatibility factors

The compatibility factors are plotted for n-type materials in the figure 6 and for the p-type materials in the figure 7. These curves have been obtained from real measurements of the Seebeck coefficient, thermal and electrical conductivities of the thermoelectric materials.

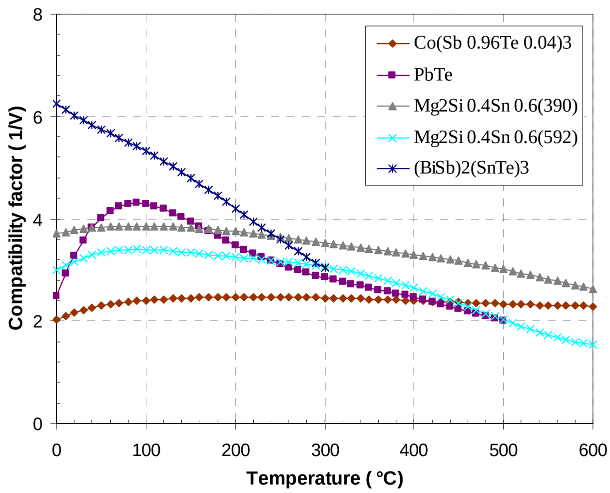

Figure 6: Compatibility factors for n-type materials

The curves in the figure 6 shows for instance that PbTe presents a very good compatibility with Mg_2Si when the temperature of the interface of the sandwich leg is around 200°C

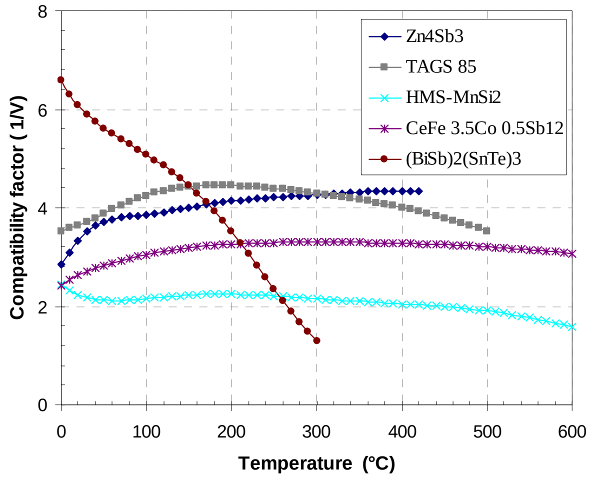

Figure 7: Compatibility factors for p-type materials

The figure 7 shows for instance that Bi_2Te_3 presents a good compatibility with Zn_4Sb_3 around 200°C.

3.2.3 Maximum of reduced efficiency

The maximum of the reduced efficiency is obtained when the relative current density is equal to compatibility factor. The expression of the maximum of the reduced efficiency is then:

$$max\,\eta_r(u) = \eta_r(s)$$

$$= \frac{1-s\frac{\alpha}{z}}{1+\frac{1}{s\alpha T}} = \frac{1-\left(\frac{\sqrt{1+zT}-1}{\alpha T}\right)\frac{\alpha}{z}}{1+\frac{1}{\left(\frac{\sqrt{1+zT}-1}{\alpha T}\right)\alpha T}} = \frac{\sqrt{1+zT}-1}{\sqrt{1+zT}+1} \tag{9}$$

The expression of the maximum of the reduced efficiency given by the equation (9) is used to plot its evolution versus temperature for different thermoelectric materials.

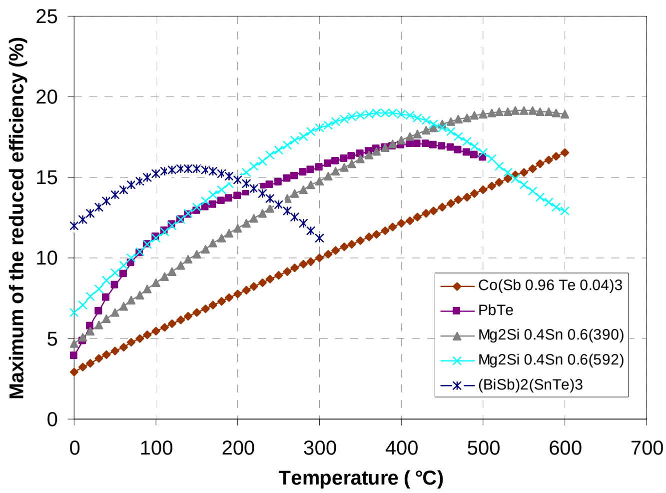

Figure 8: Maximum of the reduced efficiency for n-type materials

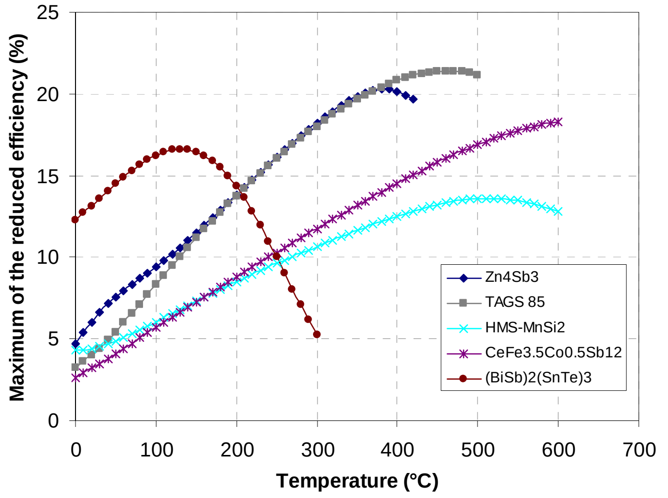

Figure 9: Maximum of the reduced efficiency for p-type materials

The curves obtained are represented for n-type thermoelectric materials in the figure 8 (respectively for p-type thermoelectric materials in the figure 9).

For instance, if the temperature of the cold side of the thermoelement is about 20°C and the hot side is about 400°C, it is obvious that the best results will be obtained with the following configuration for the thermoelement:
- a thermoelectric leg made with Bi_2Te_3 for the cold part and Zn_4Sb_3 or TAGS 85 for the hot part for the p-leg (see figure 9)
- a thermoelectric leg made with Bi_2Te_3 for the cold part and Mg_2Si for the hot part for the n-leg (see figure 8).
The best interface temperature which will give the optimized results is about 200°C.

3.2.4 Example

Let consider the case of a p-leg which must work with a cold side at ambient temperature and a hot side at 600°C. The best configuration is Bi_2Te_3 for the cold part, TAGS 85 for the hot part and an interface temperature at 200°C.

Now let determine the best operating conditions that is to say let evaluate the efficiency of the p-leg as a function of the value of the relative current density at the hot side u_h and determine which value u_h gives the best efficiency.

Several simulations are performed to obtain the curve plotted in the figure 10 (one simulation for each square mark on the curve of figure 10).
The best efficiency is obtained for u_h=4,46V and is equal to 17,38%. Moreover, the value of the efficiency decreases quickly (respectively slowly) if the value of the relative current density is too low (respectively too high).

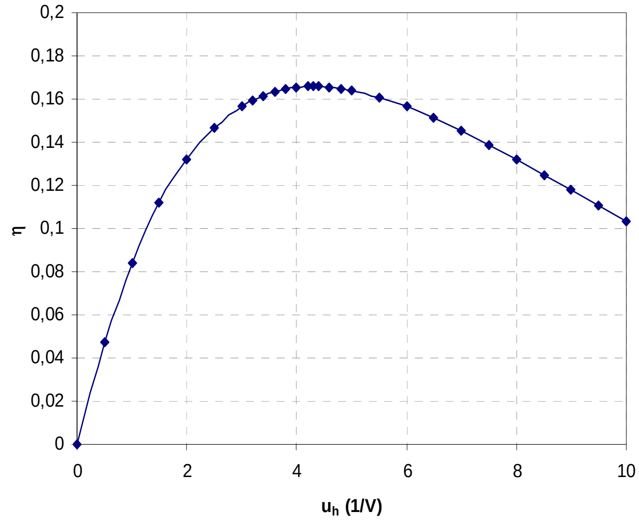

Figure 10: Efficiency as a function of the relative current density value at the hot side

Then, the influence of the cold side temperature on the efficiency of the segmented leg is investigated for three different hot side temperatures (400°C, 500°C, 600°C). The results are presented in the figure 11.

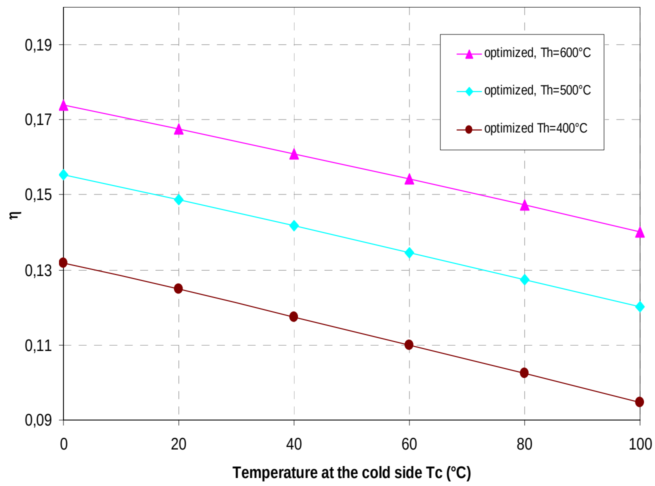

Figure 11: Influence of the cold side temperature on the efficiency of the p-leg for three different temperatures at the hot side

For a hot side temperature equal to 600°C, the efficiency decreases from 17.38% to 14.02% when the cold side temperature increases from 0°C to 100°C. For the hot side temperature equal to 500°C (respectively 400°C) the efficiency loss is 3.53% (respectively 3.71%).

4 Conclusion

In this study, modelling of the heat transfer in a thermoelement is proposed in order to have a better

understanding of the phenomena which occur and to determine the efficiency of the thermoelement. Two methods are used to solve the heat transfer equation in a thermoelectric leg: analytical and numerical.
Simulations are performed with the software FlexPde which solves partial differential equations through the finite element method. The influence of the Thomson effect and also the non linearity due to the thermodependence of the thermophysical parameters are taken into account and investigated thanks to the simulations.
Results in terms of temperature and fluxes are presented (these quantities are needed if one wants to have the coefficient of performance of the thermoelectric device). There is a good agreement between the results obtained with the analytical model and with the finite element method.
Then the case of a segmented leg (sandwiched structure) used for instance in Radioisotope Thermoelectric Generators is studied through the compatibility factors and reduced efficiency. These quantities are helpful in the design of the leg (choice of the thermoelectric materials, determination of the best interface temperature and of the best value of the relative current density).

References:

[1] B. Sherman, R. R. Heikes, and R. W. Ure, Calculation of Efficiency of Thermoelectric Devices, *Journal of Applied Physics* 31, 1, 1960.

[2] D.M. Rowe, Applications of nuclear-powered thermoelectric generators in space, *Applied Energy*, Vol. 40, No. 4, 1991, pp. 241-271.

[3] Mohamed S. El-Genk, Space nuclear reactor power system concepts with static and dynamic energy conversion, *Energy Conversion and Management*, Vol. 49, No. 3, 2008, pp. 402-411.

[4] M. Lazard, E. Rapp, H. Scherrer, Some considerations towards design and optimization of segmented thermoelectric generators, *5th European Conference on Thermoelectrics* (Odessa, Ukraine, 2007) pp. 187-191.

[5] N. Espinosa, M. Lazard, L. Aixala, H. Scherrer, Modelling TEG applied to diesel automotive heat recovery, *28th International Conference on Thermoelectrics*, (Fribourg, Germany, 2009).

[6] M. Lazard, H. Catalette, L. Lelait, H. Scherrer, Innovative use of thermoelectricity for nuclear waste: Modelling, estimation and optimization, *International Review of Mechanical Engineering*, Vol. 1, No. 4, 2007, pp. 451-462.

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

[8] D. M. Rowe, *Thermoelectric Handbook*, edited by D. M. Rowe (CRC, Boca Raton, 1995).

[9] G. Fraisse, M. Lazard, C. Goupil, J.J. Serra, Study of a thermoelement’s behaviour through a modelling based on electrical analogy, *International Journal of Heat and Mass Transfer, submitted.*

[10] M. Lazard, G. Fraisse, C Goupil, H. Scherrer, Thermal analysis of a thermoelectric leg: a way to non-conventional device design, *6th European Conference on Thermoelectrics*, (Paris, France, 2008) pp-02-15-1/4.

[11] R. Yang, G. Chen, A. R. Kumar, G. J. Snyder, J.P. Fleurial, Transient cooling of thermoelectric coolers and its applications for microdevices, *Energy Conversion and Management*, Vol. 46, N°9-10, 2005, pp 1407-1421.

[12] Swanson B. W. et al, Optimization of a Sandwiched Thermoelectric Device, *Journal of Heat Transfer*, (1961), pp. 77-82.

[13] Mohamed S. El-Genk, Hamed H. Saber and Thierry Caillat, Efficient segmented thermoelectric unicouples for space power applications, *Energy Conversion and Management*, Vol. 44, (2003), pp 1755-1772.

[14] G. J. Snyder, Design and Optimization of Compatible, Segmented Thermoelectric Generators, in Twenty-second *International Conference on Thermoelectrics*. Proceedings, ICT'03 (IEEE, La Grande Motte, France, 2003), p. 443.