Modeling of a thermoelement with segmented legs for RTG applications

M. LAZARD [1], J.P. ROUX [2], A.A. PUSTOVALOV [3], H. SCHERRER [4]
Institut PPrime UPR 3346, ENSIP, B25, Campus Sud, 2 rue Pierre Brousse, 86000 Poitiers, FRANCE
E-mail: myriam.lazard@univ-poitiers.fr
AREVA TA, Energy Systems, CS50497, 13593 Aix en Provence, FRANCE
E-mail: Jean-Pierre-Roux@technicatome.com
BIAPOS, Research-Industrial Enterprise, Leninsky prospect, 38k.1, 119334 Moscow, RUSSIAN FEDERATION
E-mail: biapos.office@g23.relcom.ru
Institut Jean Lamour, LPM, Ecole des Mines, Parc de Saurupt, CS 14 234, 54042 Nancy FRANCE
E-mail: hubert.scherrer@mines.inpl-nancy.fr

Abstract: - This study deals with the modelling of segmented thermoelements for Radioisotopic Thermoelectric Generator. One of the more important quantities for a thermoelement as well as for any device is its efficiency. As far as a thermoelement with segmented legs is concerned, it is not an easy task to evaluate its efficiency. In a first step, approximations are made and the values of the thermophysical and thermoelectrical parameters are assumed to be constant (mean values are used to perform calculi). Then a more complete modelling is proposed: the thermo dependence of the parameters is taken into account. The compatibility of the thermoelectric materials is checked and an optimization is be made in order to determine the value of the relative current density that allows to maximize the efficiency of the thermoelement.

Key-Words: - Modelling, Radioisotopic Thermoelectric Generator, segmented legs, efficiency

1 Introduction

As reported in a lot of papers, thermoelectricity is obviously an attractive way to power generation. The main advantages of thermoelectric devices summarized for instance in [1] are compactness, quietness, high reliability and environmental friendliness. Recent developments in theoretical studies as well as many efforts on elaborating new materials and on measuring their properties [2] provide many opportunities for a wide range of applications such as for instance automotive heat recovery [3], nuclear waste [4], solar thermoelectric generator [5] and last but not least space applications with the Radioisotope Thermoelectric Generators (RTG) [6-9].

RTGs work by converting heat from the natural decay of radioisotope materials into electricity; the two junctions of the thermoelement are kept at different temperatures and this temperature difference is relatively large. To achieve a better efficiency and as no single thermoelectric material presents high figure of merit over such a wide temperature range, it is therefore necessary to use different materials and to segment them together in order to have a sandwiched structure [10, 11]. In this way, materials are operating in their most efficient temperature range.

In this paper, we present the modelling of thermoelectric segmented legs to be used for RTG. The aim is to calculate their efficiency and to determine the best operating conditions. After a rough estimation of the efficiency with considering mean values for the thermophysical properties, a complete modelling is proposed with taking the thermodependence of the coefficients into account. Data used for the modelling are obtained from measurements and are fitted by curves in order to have a more accurate modelling. Quantities such as compatibility factors, reduced efficiency are plotted as function of temperature or of relative current density which is the ratio of the electric current density to the heat flux by conduction. Another configuration with other thermoelectric materials is also investigated and the influence of the temperature at the cold junction is also discussed.

2 Configuration and rough estimation of the efficiency of the thermoelement

2.1 Configuration of the thermoelectric leg

The figure 1 shows the case studied in this paper. It corresponds to a couple of thermoelectric elements of N-type and P-type.

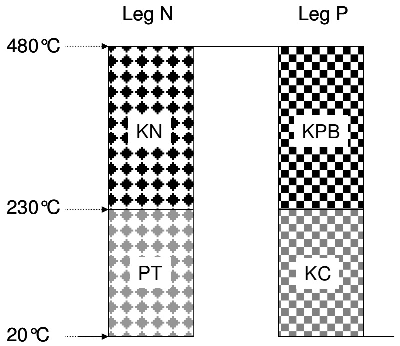

Fig.1: Scheme of the segmented thermoelement

For the N_leg, the "Hot" segment is alloy KN (PbTe + 0.04% mol PbI2+ 1.5% Pb) and the "Cold" Segment is alloy PT (PbTe + 0.016% mol PbI2+ 1.5% Pb)
For the P_leg, the "Hot" segment is alloy KPB (97% GeTe + 3% BiTe+ 2% Cu) and the "Cold" Segment is alloy KC (26% mol Bi2Te3+ 74% mol Sb2Te3 + 0.17%wgt Pb + 3% wgt Te)
The cold temperature is 20°C, the hot temperature 480°C and the interface temperature between the segments is 230°C.

2.2 Approximate efficiency of a segmented thermoelement

In the case of segmented legs with different thermoelectric materials, the thermophysical and thermoelectric properties are different. To have an idea of the maximum of the efficiency, it is necessary as a first approach to take the mean of these values. Then a more accurate and more complete modelling will be made in order to check if it is interesting to segment the materials together (that is to say if they are compatible).
The mean values chosen are those summarized in the table 1.

Table 1: Mean values of the thermoelectric properties of the materials

	Seebeck Coefficient $V/K\,10^{-6}$	Thermal conductivity $W/cm.K\,10^{-2}$	Electrical resistivity $\Omega.cm\,10^{-4}$
KN	219.8	1.4	26.58
PT	223.5	2.2	16.76
mean	***221.65***	***1.8***	***21.67***
KPB	200.44	2.09	13.65
KC	184.7	1.544	12.66
mean	***192.57***	***1.817***	***13.155***

Two different equations could then be used to evaluate the factor of merit Z_{pn}

$$\overline{Z}_{pn} = \frac{Z_n + Z_p}{2} \text{ with } Z_i = \frac{\alpha_i^2}{\rho_i \lambda_i} \quad (1)$$

$$Z_{pn} = \left[\frac{\alpha_{pn}}{(\rho_n \lambda_n)^{1/2} + (\rho_p \lambda_p)^{1/2}} \right]^2 \quad (2)$$

Where α is the Seebeck coefficient, ρ is the electrical resistivity, λ is the thermal conductivity and the upperscript i is n for the N_leg (respectively p for the P_leg).

With the data of the table 1, it gives:

$$\overline{Z}_{pn} \approx 1.405472292\ 10^{-3}\ K^{-1}$$

$$Z_{pn} \approx 1.3840677410^{-3}\ K^{-1}$$

It leads to a rough estimation of an approximate efficiency by using the following equations [12]:

$$\omega = (1+Z_{pn}\,\overline{T})^{1/2} \text{ with } \overline{T} = (T_f + T_c)/2 \quad (3)$$

$$\eta_{max} = \frac{\Delta T}{T_c} \frac{\omega - 1}{\omega + T_f/T_c} \quad (4)$$

Finally, the approximations of the maximum of the efficiency is :

$$\eta_{max}(\overline{Z}_{pn}) \approx 11.35\%$$

$$\eta_{max}(Z_{pn}) \approx 11.23\%$$

2.3 Example of a segmented leg

As every thermoelectric material presents a figure of merit more or less high depending on the temperature range, when the device is used for a large range of temperature, it is interesting to consider a segmented leg: each segment is constituted by a thermoelectric material which has high figure of merit for the intermediate ranges of temperature considered [10].
Some important quantities are needed to investigate a segmented leg such as for instance the relative current density or the compatibility factor [13, 14] and also the maximum of the reduced efficiency and the reduced efficiency.
Let first consider the relative current density that goes through the segmented leg. It is plotted in the figure 2 as a function of the temperature.

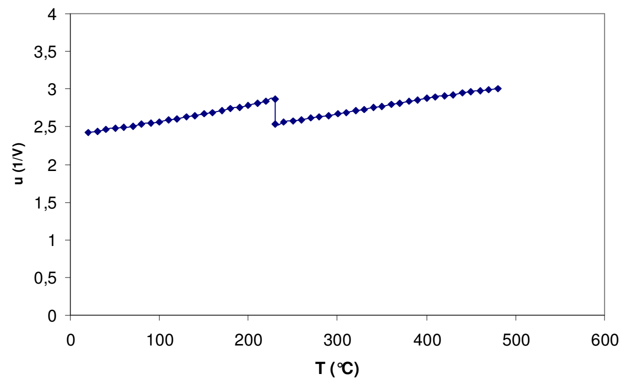

Fig. 2: Evolution of the relative current density as a function of the temperature for the segmented N-leg made with KN and PT

The variations of the relative current density are not so important because they are between 2.4 V^{-1} and 3 V^{-1} (relative variation less than 25%). The "jump" of the relative current density corresponds to the interface between the two thermoelectric materials.

Let consider in the figure 3 the variation of the compatibility factor along the leg as a function of the temperature.

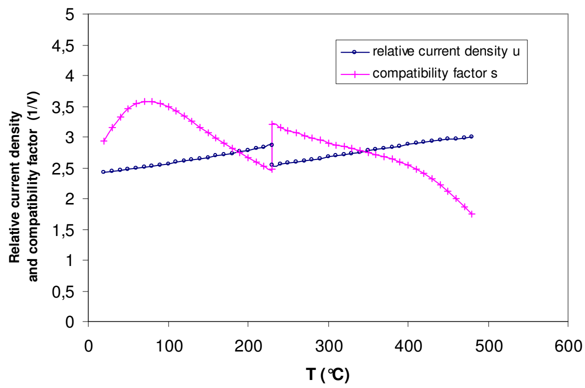

Fig. 3: Comparison between the relative current density and the compatibility factor as a function of the temperature for the N_leg (2 segments : KN and PT)

One can expect that the reduced efficiency will be a little bit lower than the maximum of the reduced efficiency (especially for the hot side of the hot segment). Let check this remark by plotting the reduced efficiency compared with the maximum of the reduced efficiency.

From the evolution of the compatibility factor as a function of the temperature within the segmented leg (respectively the relative current density), the evolution of the maximum of the reduced efficiency (respectively of the reduced efficiency) could be plotted in figure 4. The reduced efficiency is between 6,12% and 16,67%. The remark made previously is correct. In fact, the real reduced efficiency is a little bit lower than the maximum of the reduced efficiency but nevertheless the reduced efficiency is very close to the maximum of the reduced efficiency.

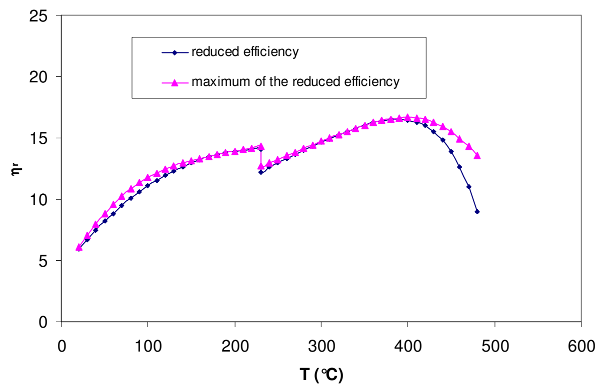

Fig. 4: Comparison between the reduced efficiency and the maximum of the reduced efficiency for the N-leg (2 segments KN and PT)

The example of a segmented leg has been investigated by considering:
- the evolution of the relative current density going through the leg compared to the compatibility factor,
- the reduced efficiency compared with the maximum of the reduced efficiency

Now, the attention will be focused on results dealing with the core of the problem that is to say the efficiency of a segmented leg. It is not an easy task because the relative current density varies along the leg (because it depends on the temperature and the temperature varies along the leg). An optimization is performed in order to determine the best values of the relative current density at the hot side which will allow to obtain the best efficiency.

3 Modelling the thermoelement and its efficiency

3.1 Relevance of the configuration

The chosen configuration presented previously is relevant because KN is compatible with PT and KPB is compatible with KC. The figures 5a and 5b proved it: they present the compatibility factors of the materials whose values are summarized in the table 2.

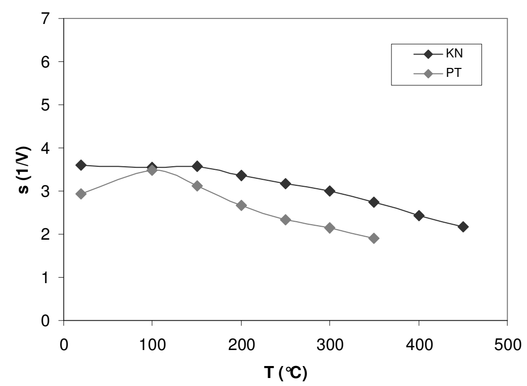

Fig. 5 a: Compatibility factors for the materials of the N-leg

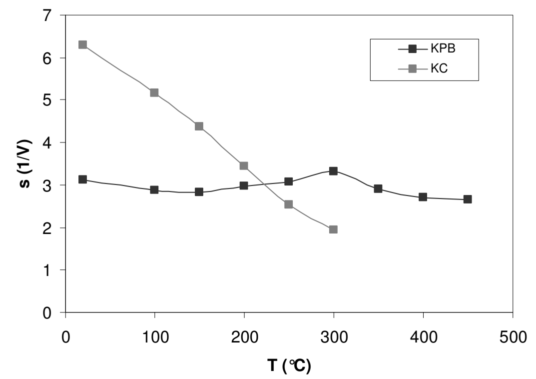

Fig. 5 b: Compatibility factors for the materials of the P-leg

Table 2: Values of the compatibility factors depending on the temperature for the materials KN, PT, KPB et KC

	LEG N		LEG P	
	KN	PT	KPB	KC
T (°C)	s (1/V)	s (1/V)	s (1/V)	s (1/V)
20	3,589664	2,92885	3,121085	6,291563
100	3,543983	3,483041	2,880174	5,157701
150	3,564295	3,111577	2,829251	4,380882
200	3,351479	2,65887	2,964529	3,426604
250	3,166395	2,323069	3,068736	2,539418
300	3,000800	2,135204	3,305652	1,937861
350	2,742982	1,907341	2,903932	
400	2,428441		2,697266	
450	2,155773		2,643462	

Indeed, the values of the compatibility factors of KN and PT are very close to each other (see figure 5a). It allows to affirm that the segmentation is relevant and efficient and that it will be possible to find a relative current density that will be suitable for KN and PT. As a consequence, it allows to obtain an optimal efficiency close to the maximum efficiency.

On the other hand, the compatibility factor of KC is higher than compatibility the factor of KPB but only for the cold temperatures. A priori, it could be a drawback but in fact it is not the case as far as the curves of the compatibility factors of KC and KPB are intersecting and the point of this intersection will be chosen as the temperature of the interface between the two thermoelectric materials.

3.2 Some comments before the evaluation of the efficiency and the optimization

The Seebeck coefficient, the thermal conductivity and the electrical resistivity are needed for the modelling that is why they are real values obtained by measurements performed for several temperatures (from the ambient and each fifty degrees).
On the other hand, in order to have a complete and accurate modelling, one must have the values not each 50°C but every 10°C. The experimental points must be fitted by curves.

Some examples of the curves representing the Seebeck coefficient, the thermal conductivity and the electrical electricity are plotted for KN and PT in the figures 6, 7, 8.

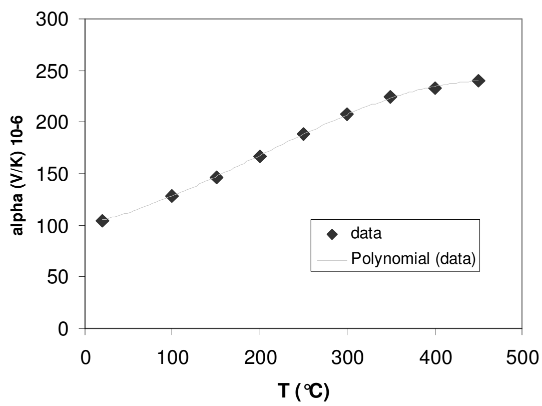

Fig. 6 a: Seebeck coefficient of KN (data from measurements and curves from fitting)

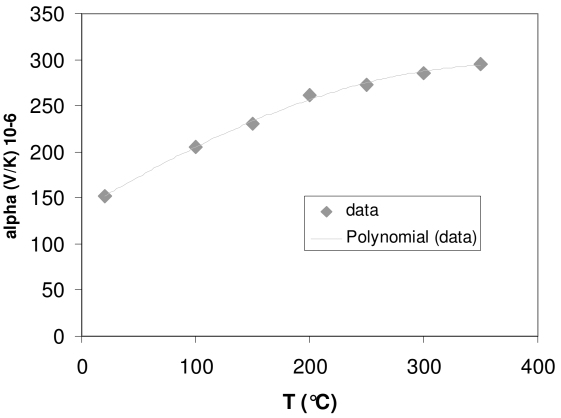

Fig. 6 b: Seebeck coefficient of PT (data from measurements and curves from fitting)

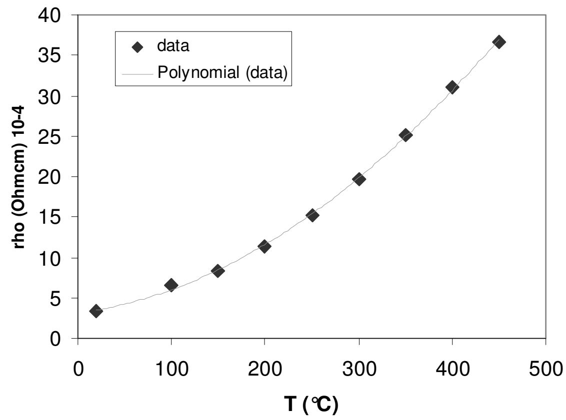

Fig. 8 a: Electrical resistivity of KN (data from measurements and curves from fitting)

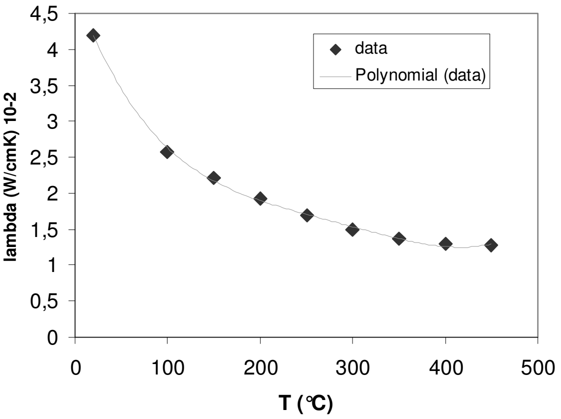

Fig. 7 a: Thermal conductivity of KN (data from measurements and curves from fitting)

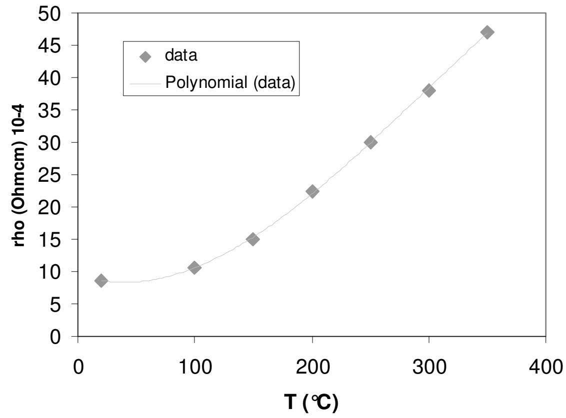

Fig. 8 b: Electrical resistivity of PT (data from measurements and curves from fitting)

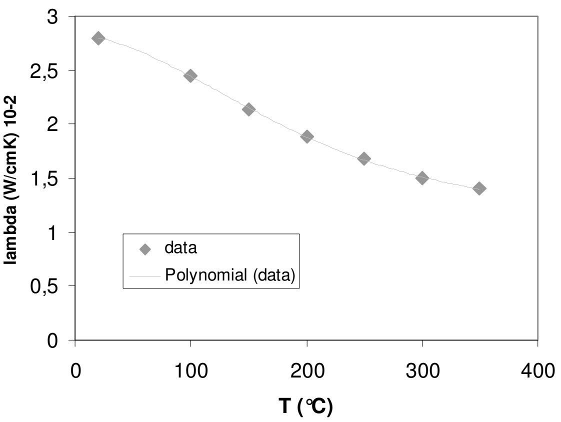

Fig. 7 b: Thermal conductivity of PT (data from measurements and curves from fitting)

As far as the factor of merit ZT is concerned, there are two possibilities to obtain the corresponding curves:

- either ZT is evaluated every 50°C from the experimental values of α,λ,ρ every 50°C and then the curves are plotted from these points corresponding to ZT every 50°C
- either ZT is obtained from the fitted curves of α,λ,ρ

It is this last solution which is chosen for the calculations because it allows to have more accurate results (the figure of merit corresponds better to the values obtained from the experimental values –see figures 9a and 9b).

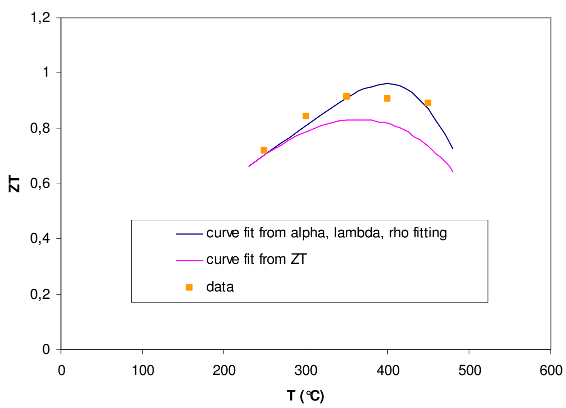

Fig. 9 a: Figure of Merit of KN

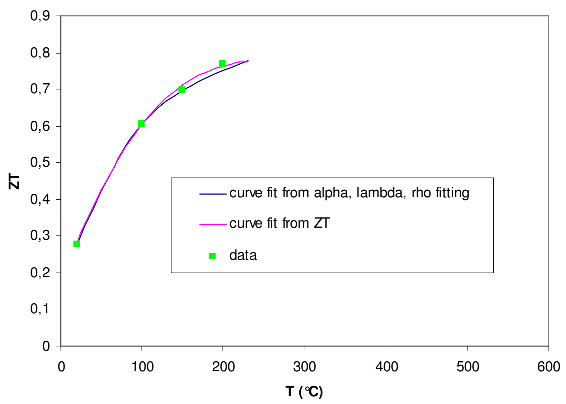

Fig. 9 b: Figure of Merit of PT

3.3 Study of the P-leg

The efficiency η which is a fundamental quantity is function of the relative current density u which is itself solution of a differential equation [14]. With all the quantities needed, the efficiency is calculated with Excel for a segmented leg for several values of the relative current density at the hot side uc (and so for several relative current densities going through the leg). The results are presented in the figure 10.

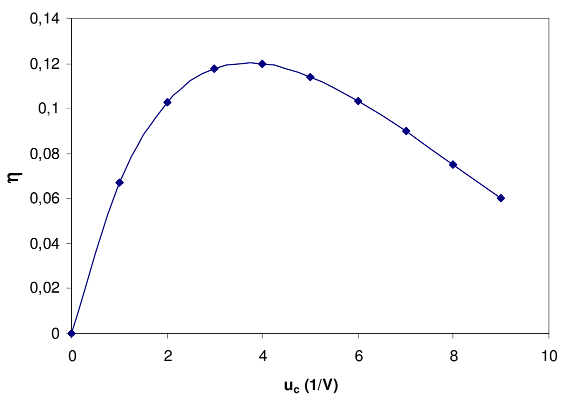

Fig. 10: Efficiency of the P_leg as a function of the relative current density u_c

When there is a thermal gradient equal to 460°C (TC=480°C, TF=20°C): for the P_leg, after optimization of the value of the relative current density at the hot side, the optimal efficiency is 12,01 % and is obtained for uc=3,70 V^{-1}.

It is also interesting to consider the evolution of the relative current density within the leg as function of the temperature (figure 11) and to compare it with the compatibility factor. In the figure 12, the reduced efficiency and the maximum of the reduced efficiency are compared.

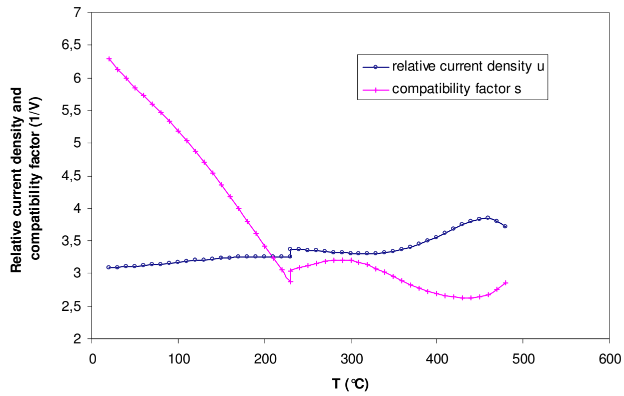

Fig. 11: The relative current density and the compatibility factor as functions of the temperature within the segmented leg

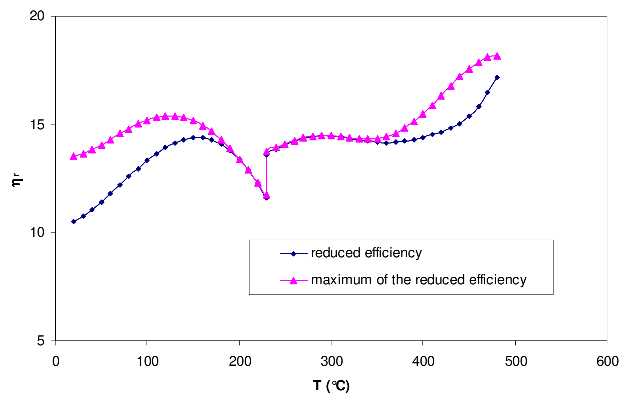

Fig. 12: Reduced efficiency and maximum of the reduced efficiency as functions of the temperature

The relative current density does not vary a lot and the reduced efficiency obtained from this relative current density that goes through the leg is close to the maximum of the reduced efficiency (it is for the extreme points that the difference is the highest).
The optimization performed which consisted in maximizing the value of the efficiency by taking the variable parameter u_c gives satisfactory results.
The efficiency of the P_leg is now known, let consider now the case of the N_leg.

The same analysis will be made but the curves corresponding to the relative current density and the reduced efficiency will not be presented because they have already been presented in the section "example of a segmented leg".

3.4 Study of the N-leg

The efficiency η is presented as a function of the relative current density at the hot side in the figure 13.

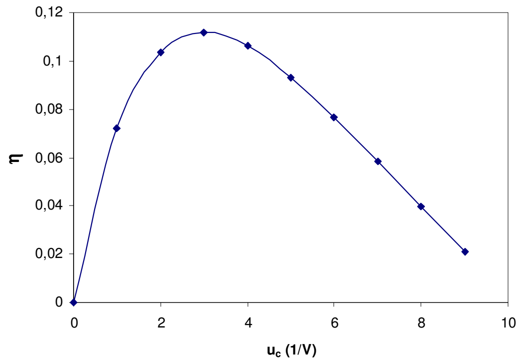

Fig. 13: Efficiency of the N_leg as a function of the relative current density u_c

When there is a thermal gradient equal to 460°C (TC=480°C, TF=20°C), for the N_leg, after optimization of the value of the relative current density at the hot side, the optimal efficiency is 11.17% and is obtained for u_c=2.99V^{-1}.

3.5 The efficiency of the thermoelectric generator

The efficiency of the thermoelectric generator depends on the efficiency of the N_leg and of the P_leg [15]. The equation which gives it expression is:

$$\eta = \frac{\eta_p Q_p + \eta_n Q_n}{Q_p + Q_n} \tag{5}$$

It could also be written [15]:

$$\eta = 1 - \frac{\alpha_{p,f} T_F + \frac{1}{u_{p,f}} - \alpha_{n,f} T_F - \frac{1}{u_{n,f}}}{\alpha_{p,c} T_C + \frac{1}{u_{p,c}} - \alpha_{n,c} T_C - \frac{1}{u_{n,c}}} \tag{6}$$

$$= 1 - \frac{(\alpha_{p,f} - \alpha_{n,f}) T_F + \frac{1}{u_{p,f}} - \frac{1}{u_{n,f}}}{(\alpha_{p,c} - \alpha_{n,c}) T_C + \frac{1}{u_{p,c}} - \frac{1}{u_{n,c}}}$$

For 20-480°C, the efficiency of the thermoelectric generator made with KN and PT for the N_leg and KPB and KC for the P_leg is 11.55% with the optimized values given in the table 3.

Table 3: Evaluation of the thermoelement efficiency (T cold=20°C)

Leg P			Leg N		
alpha hot	T hot	u hot	alpha hot	T hot	u hot
205,87	753	3,70	239,62	753	2,99
alpha cold	T cold	u cold	alpha cold	T cold	u cold
169,95	293	3,08	151,71	293	2,42
Thermoelement efficiency :					
0,1155					

3.6 Influence of the temperature at the cold side

The efficiency depends obviously on the gradient temperature in the leg. To investigate the influence of the temperature at the cold side (sometimes, it is difficult to cool the cold junction and to maintain it at a temperature equal to 20°C) the new temperature of the cold side is now equal to 40°C.

New calculations are performed such as for instance the relative current density and then the efficiency as function of the relative current density could be plotted for the N_leg in the figure 14a (respectively for the P_leg in the figure 14b).

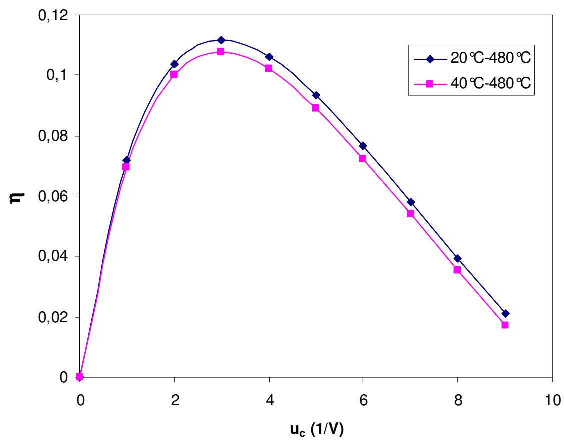

Fig. 14 a: Efficiency of the N_leg as a function of the relative current density uc(T cold=20°C or T cold=40°C)

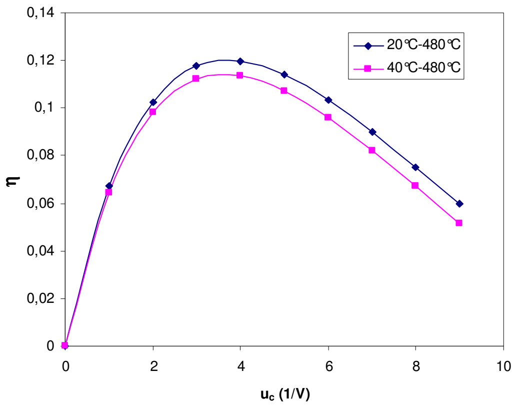

Fig. 14 b: Efficiency of the P_leg as a function of the relative current density u_c(T cold=20°C or T cold=40°C)

The curve presents the same shape but the efficiency is lower. The results are summarized in the table 4.

Table 4: Influence of the temperature on the efficiency

Value of the efficiency after optimization			
Leg P		Leg N	
20°C-480°C	40°C-480°C	20°C-480°C	40°C-480°C
12,01%	11,39%	11.17%	10,77%
Value of the relative current density at the hot side which gives the optimal value of the efficiency			
u_c=3,70 V^{-1}	u_c=3,62 V^{-1}	u_c=2,99 V^{-1}	u_c=2,97 V^{-1}

The efficiency decreases from 11.17% to 10.77 % for the N_leg which corresponds to a loss of about 0.4 % (respectively from 12.01 % to 11.39 % for the P_leg which corresponds to a loss of about 0.6 %). The new efficiency of the thermoelement is calculated with the values summarized in the table 5 and is 11.05% (instead of 11.55%).

Table 5: Evaluation of the thermoelement efficiency (T cold=40°C)

Leg P			Leg N		
alpha hot	T hot	u hot	alpha hot	T hot	u hot
205,87	753	3,6268	239,62	753	2,9742
alpha cold	T cold	u cold	alpha cold	T cold	u cold
171,35	313	3,0485	165,95	313	2,4447

Thermoelement efficiency :

0,11057

4 Configurations with other thermoelectric materials

Let now consider another configuration with other thermoelectric materials (see figure 15). The configuration chosen involves materials which are compatible together and that present a high figure of merit for each range of temperature considered.
For the N_leg, the "Hot" segment is Mg2 Si0.4 Sn0.6 and the "Cold" Segment is n-(Bi, Sb)2 (Sn,Te)3
For the P_leg, the "Hot" segment is TAGs and the "Cold" Segment is p-(Bi, Sb)2 (Sn,Te)3
The cold temperature is 20°C, the hot temperature 480°C and the interface temperature between the segments is 200°C.

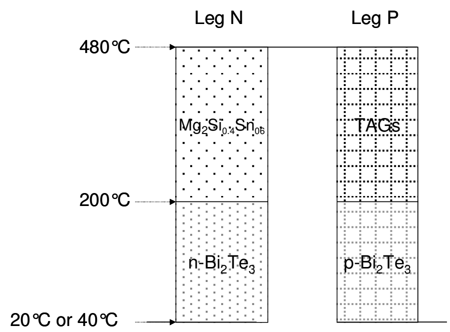

Fig. 15: Scheme of the segmented thermoelement (other thermoelectric materials)

New calculations must be performed in order to determine the intermediate quantities such as the relative current density along each leg and also the reduced efficiency. Then the most important quantity which is of course the efficiency is represented in figure 16a for the N_leg and in figure 16b for the P_leg. The shape of the curves is the same as presented in the figures 10, 13 14a and 14b. The main difference is that the maximum obtained is higher for this configuration. The exact values of the efficiencies are summarized in the table 6.

Table 6: Influence of the temperature on the efficiency for other thermoelectric materials

Value of the efficiency after optimization			
Leg P		Leg N	
20°C-480°C	40°C-480°C	20°C-480°C	40°C-480°C
14.43%	13.73%	12.77%	12.20%
Value of the relative current density at the hot side which gives the optimal value of the efficiency			
u_c=4,83 V^{-1}	u_c=4,75 V^{-1}	u_c=3,55 V^{-1}	u_c=3,48 V^{-1}

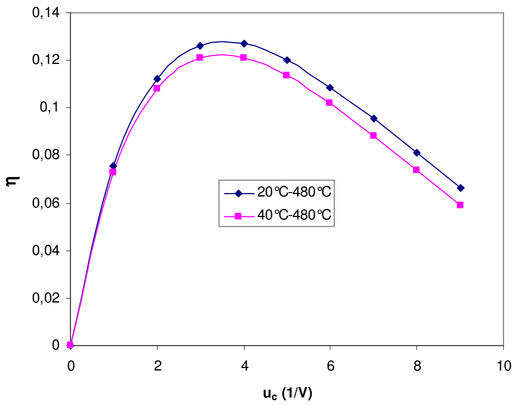

Fig. 16 a: Efficiency of the N_leg as a function of the relative current density uc (other thermoelectric materials)

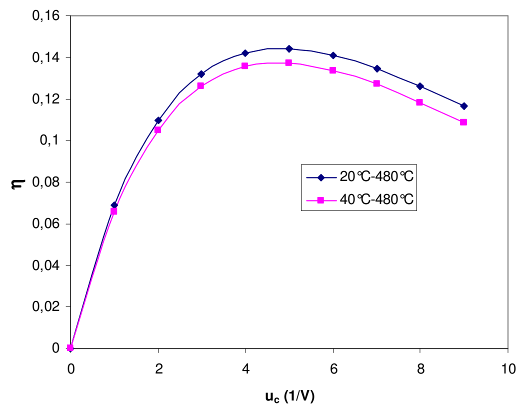

Fig. 16 b: Efficiency of the P_leg as a function of the relative current density uc (other thermoelectric materials)

For the P_leg, the efficiency is 14.43% instead of 12.01% for the previous configuration when the cold temperature is equal to 20°C (gain of 2.46%).
For the N_leg, the efficiency is 12.77% instead of 11.17% for the previous configuration when the cold temperature is equal to 20°C (gain of 1.6%).
The influence of the cold side temperature is also investigated. For the P_leg the efficiency loss is 0.57% and respectively 0.7% for the N_leg when the cold temperature is equal to 40°C instead of 20°C. These losses are more important than for the previous configuration but the efficiencies still remain higher.

The global efficiency of the thermoelement is 13.48% evaluated with the values calculated and summarized in the table 7 when the cold temperature is equal to 20°C (respectively 12.86% with the values in the table 8 when the cold temperature is equal to 40°C).

Table 7: Evaluation of the thermoelement efficiency (T cold=20°C) for other thermoelectric materials

Leg P			Leg N		
alpha hot	T hot	u hot	alpha hot	T hot	u hot
197,95	753	4,8360	239,62	753	2,9742
alpha cold	T cold	u cold	alpha cold	T cold	u cold
169,78	293	3,9257	165,95	313	2,4447
Thermoelement efficiency :					
0,1348					

Table 8: Evaluation of the thermoelement efficiency (T cold=40°C) for other thermoelectric materials

Leg P			Leg N		
alpha hot	T hot	u hot	alpha hot	T hot	u hot
197,95	753	4,7587	256,92	753	3,4810
alpha cold	T cold	u cold	alpha cold	T cold	u cold
181,56	313	3,9520	171,75	313	2,7153
Thermoelement efficiency :					
0,1286					

4 Conclusion

In this paper, a complete modelling of segmented thermoelectric legs for Radioisotope Thermoelectric Generators applications has been proposed. The operating conditions such as the temperatures at the junctions are those corresponding to RTGs conditions. The aim is to determine the efficiency of the legs and then of the thermoelement to choose the best configuration. Important quantities such as the relative current density are determined and the efficiency is evaluated as a function of the relative current density. The influence of the temperature at the cold junction on the efficiency is also investigated (when the thermal gradient at the both sides of the thermoelement decreases in 20°C, the efficiency decreases in about 0.5% - 1%). Another configuration with other thermoelectric materials is proposed and the efficiency obtained in this case is higher than those obtained previously.

No doubt, this modelling is only theoretical but it allows to obtain an estimation of the efficiency of the thermoelement and to test several configurations (materials, boundary conditions) and to see their impact on the efficiency. Moreover the thermodependence of the thermophysical properties such as the Seebeck coefficient, the thermal conductivity and the electrical resistivity which have been measured is taken into account. Of course, experimental tests will still remain the best way to see if the efficiency calculated from the modelling with the simulations corresponds to the real case. Nevertheless, this modelling is helpful to design an efficient segmented thermoelement and to find the best operating conditions.

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