Thermoelectric Generator Design and Simulation Guide

Alberto Ferrario

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Overview

TeGDS is a program to easily simulate and analyse the performance of a thermoelectric generator as a function of temperature, by describing the temperature dependent material properties, the geometry and other interface materials. The program uses an iterative algorithm that, starting from external temperatures, evaluate the temperature losses in passive elements and corrects the effective temperatures on thermoelectric elements.

This simulation tool can be used to compare experimental data of new or commercial module in operating conditions or to study the effects of interface layers. It is also useful to design a thermoelectric generator with new material data and to optimize the geometry by adjusting the parameters.

Details of the code are described in the following article:

https://doi.org/10.1016/j.applthermaleng.2019.01.031
(https://www.sciencedirect.com/science/article/pii/S1359431118353298?dgcid=author)

Note: the following steps guide the User to the design of a TE module and the simulation of its properties as a function of temperature. They are not intended to provide concepts or equations on thermoelectric physics.

Note: Application version: 2.6;

1 – File path

In the **Convergence & Output** tab choose the file path. This path indicates the folder where results will be saved and user material data stored and recovered. (Configuration and geometry files will be added in a next update).

2 - Material Properties

Enter the **Thermoelectric Properties** tab. Insert Seebeck coefficient (α), thermal conductivity (κ) and electrical conductivity (σ) as a function of temperature of n-type or p-type materials. Available are predefined values from literature. It is possible to insert user material properties in three ways:

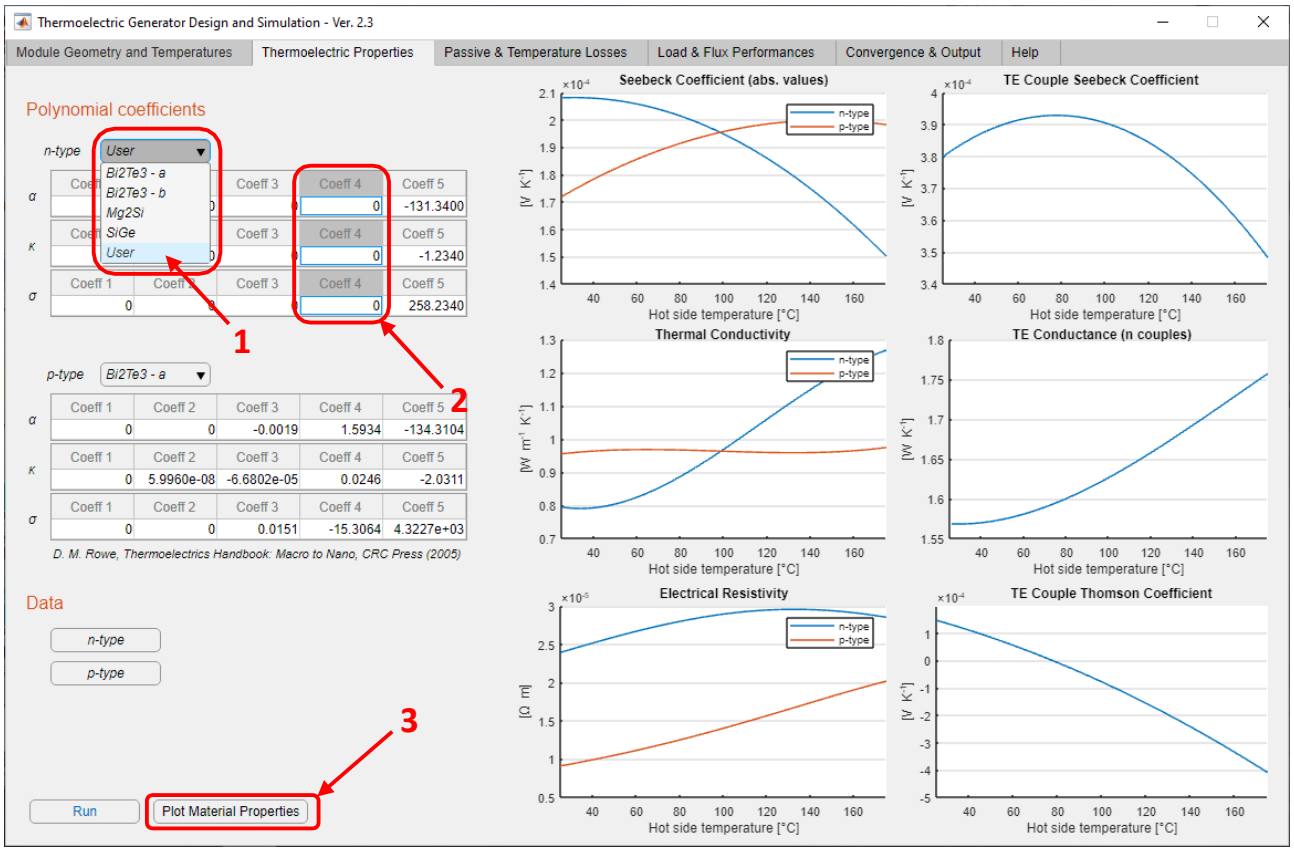
2.1 - With Polynomial coefficients

Choose **User** option from *n-type* drop-down menu (1). Table will show all zero values. In each item enter the corresponding coefficient (2) of a 4th degree polynomial in the following form

Coeff 1 x^4 + Coeff 2 x^3 + Coeff 3 x^2 + Coeff 4 x + Coeff 5.

With 2nd degree (and 1st degree) polynomial, Coeff 1 and Coeff 2 (and Coeff 3) will be zero.

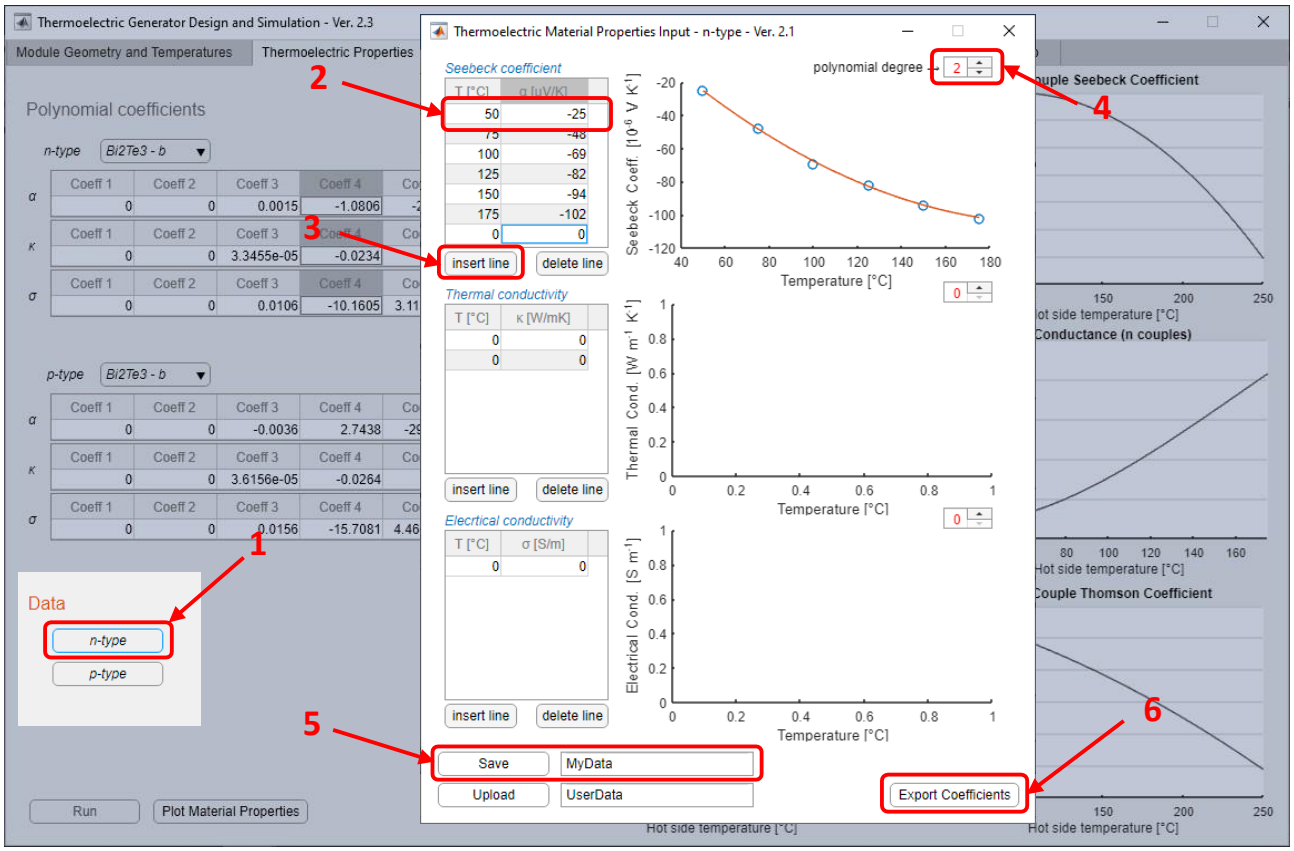
Repeat the procedure for p-type material, the push **Plot Material Properties** button (3). Material properties as a function of temperature are shown on left plots. Additional, Seebeck and Thomson values are calculated for a TE couple (right).



2.2 - With material **Data**

In case you have experimental data of your material, or literature data, as a function of temperature, push **n-type** (or p-type) button (1). A new window will open. Type experimental data in corresponding table (2). Push **insert line** button (3) to add new values. Data points will be added in the graph on the right. Once all data have been inserted, choose the degree (4) of fitting polynomial (usually 1 or 2 is good). Then save data (5) with a proper name (avoid space and reserved chars). Finally export the coefficients obtain from fitting (6). They will be automatically uploaded in the polynomial coefficients table.

Repeat the procedure with p-type data.



2.3 - With material **data file**

User material data can be uploaded from previously saved file (2.2-5). Open the input data window (1), insert the name of data file and push upload button (2). Then set the polynomial degree (3) and export coefficients (4).

Repeat the procedure with p-type data.

User data file can be created in the following form:

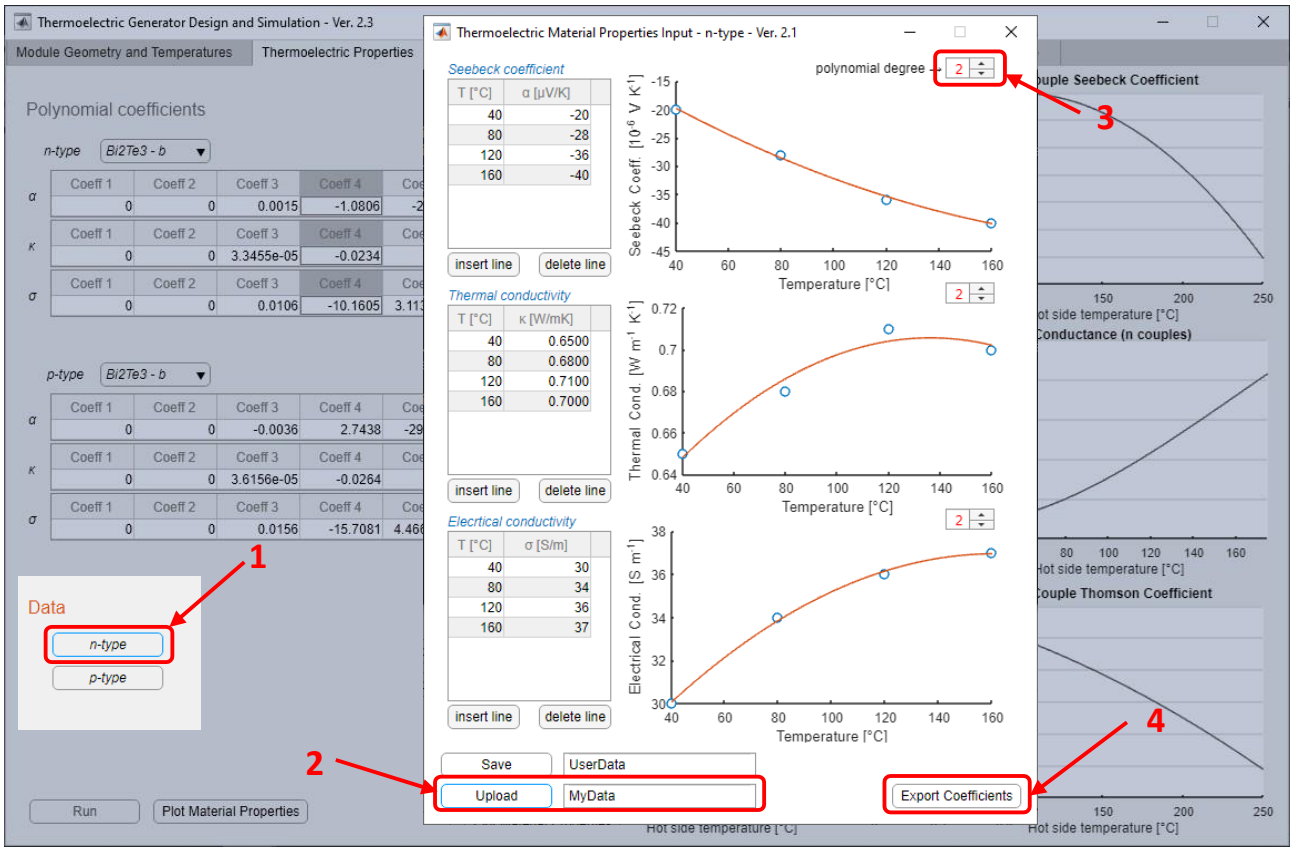
```
x1 Var2
40 -20
80 -28
120 -36
160 -40
```

Where `x1` is the temperature column and `Var2` the thermoelectric data column. File must be saved with the following names:

```
MyData-an  MyData-ap
MyData-kn  MyData-kp
MyData-sn  MyData-sp
```

Where `a`, `k` and `s` mean Seebeck coefficient [10e-6 V K-1], thermal conductivity [W m-1 K-1] and electrical resistivity [S m-1] respectively. Temperatures are in °C.

The suffix –xy will be automatically added when saving files from data input window (Sec. 2.2).



Once material properties are loaded with step 2.2 or 2.3, temperatures range will automatically update from data. If material properties are loaded with polynomial coefficients, temperatures range must be manually set.

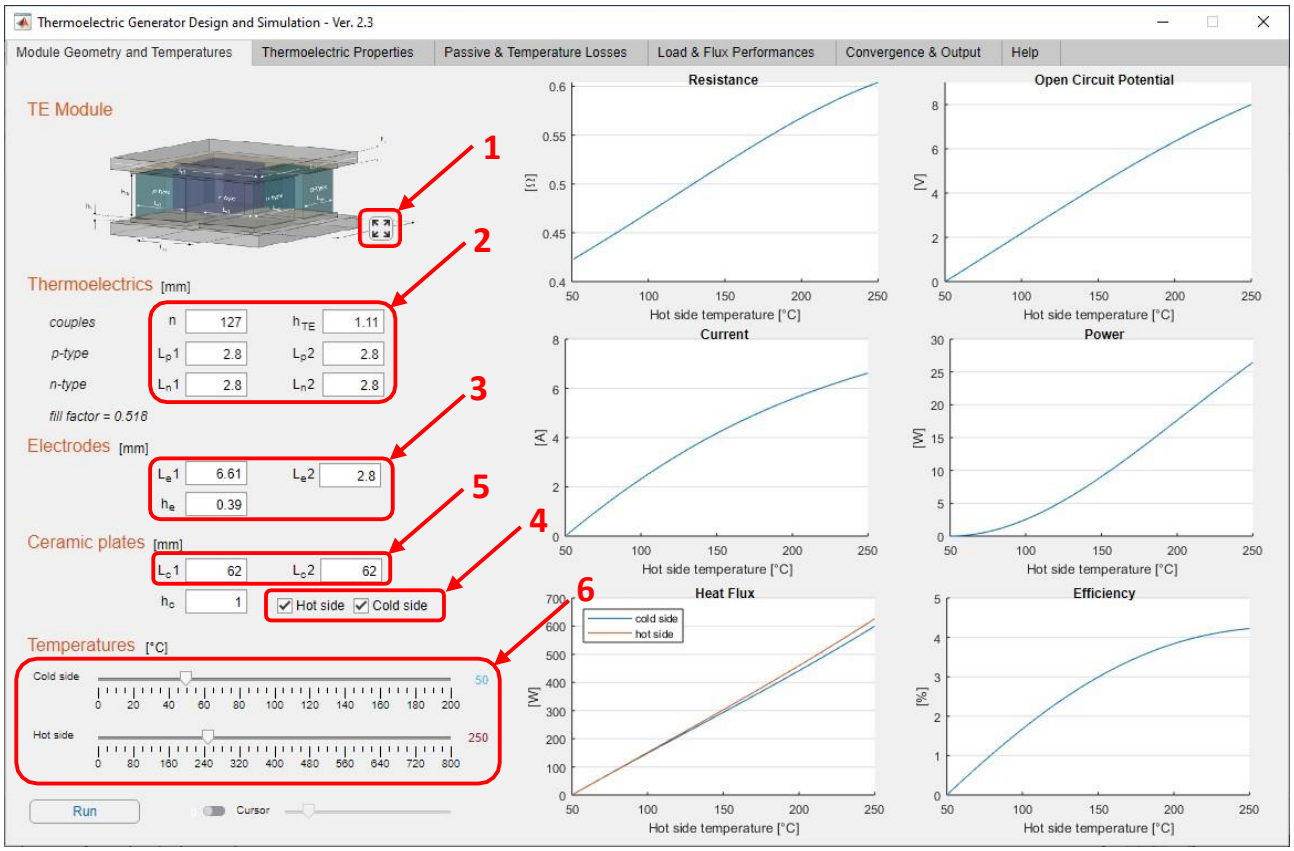
3 – Geometry

Enter the **Module Geometry and Temperatures** window to set main dimensions of thermoelectric module. Press the expand button (1) to enlarge the simplified drawing of a module. Parameters of active elements (2) are the number of couples (*n*), n-type and p-type elements dimensions (*Ln1*, *Ln2*, *Lp1*, *Lp2*) and height (*hTE*). Electrode sizes (*Le1*, *Le2*) should be at least as the sum of TE elements lengths, while the height (*he*) should minimize the electrical resistance (in particular with high current values)(3). Ceramic plates acts as substrates and insulators, they can be applied on one or both cold and hot sides by selecting the proper flag (4). Sides (*Lc1*, *Lc2*) must be set in order to guarantee an area higher than the overall TE elements area (5). Height (*hc*) should not be higher than TE elements height to minimize thermal losses.

The program checks *only* basic size constraints: 1) Overall TE active area is larger than passives area. 2) Area of a p-n couple is larger than electrode area. 3) maximum of n-type or p-type dimensions is larger than minimum of electrode dimensions. User is supposed to verify all geometric constrains.

Note: thought basic constraints must be guarantee, the code is based on a 1D model, thus overall characteristics are effective.

Finally set minimum cold side (*Tc*) and maximum hot side (*Th*) temperatures in °C with the slide bars (6). Iterations will be performed from *Tc* up to *Th*. Be aware to set a temperature range compatible with material data. Outside this range, calculations are not consistent.



4 – Passives

Passives determine most of thermal losses. They are components of a TE module (ceramic plates, electrode) or secondary elements which are used in real application (i.e. thermal layer, paste, glue, heat exchangers, etc.). Each can be characterized by a thermal resistance. **Passive & thermal losses** tab is dedicated to this.

Ceramic plates material (dimensions are set in Sec. 3) can be choose from the drop-down menu. Common used materials are preloaded: Al2O3 with 10% porosity, AlN and SiC. For different material choose **User** option and insert polynomial coefficients as explained in 2.1. Push **Plot Material Properties** button. Ceramic thermal conductivity as a function of temperature is shown in the top-left plot.

Electrodes material can be chosen from a drop-down menu from a set of materials: Cu, Ni, Al. Select **User** option to set different material properties. Insert thermal conductivity [W m-1 K-1] at room temperature, electrical resistivity [Ω m] at room temperature and the temperature coefficient of resistivity. If the specific

contact resistivity [Ω cm^2] is known experimentally or from literature. If not choose the default value or lower. Values higher than 10^5 Ω cm^2 can strongly affect the overall electrical resistance and performances.

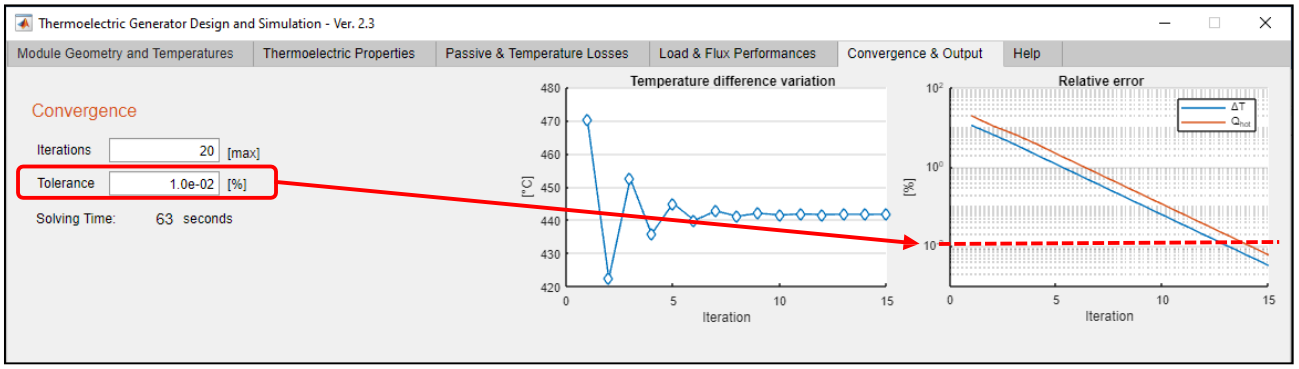
Additional thermal interfaces can be added. Each can be applied on one or both cold and hot sides by selecting the proper flag. Then insert thermal conductivity [W m-1 K-1] value and height [mm]. **Note:** avoid external layers for the first simulation, add them gradually to understand their impact on overall results.

Push **Plot Material Properties** button. Overall passive thermal conductance as a function of temperature is shown in the top-right plot.

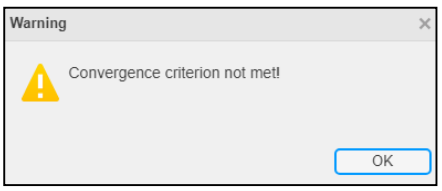
5 – Execute Simulation and Convergence

Once set all material properties and geometry, push **Run** button from any tab and wait the end of the progress bar. The command window shows the progress of iterations. Depending on PC hardware and TE module configuration, the process can take from few seconds up to few minutes.

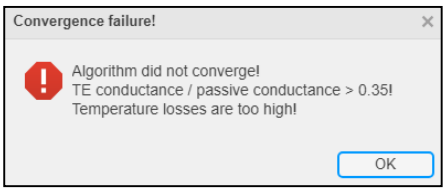
Once the simulation is finished check the convergence (**Convergence & Output**). If no warning comes out, relative error of temperature difference (ΔT) and heat flux at hot side (right plot), at the end of iterative process, is below the set tolerance value [%] (default is 10^{-2} %). Left plot shows the internal temperature difference (temperature difference at the TE elements) calculated and updated as a function of iteration number (starting value is not shown), at maximum hot side temperature.



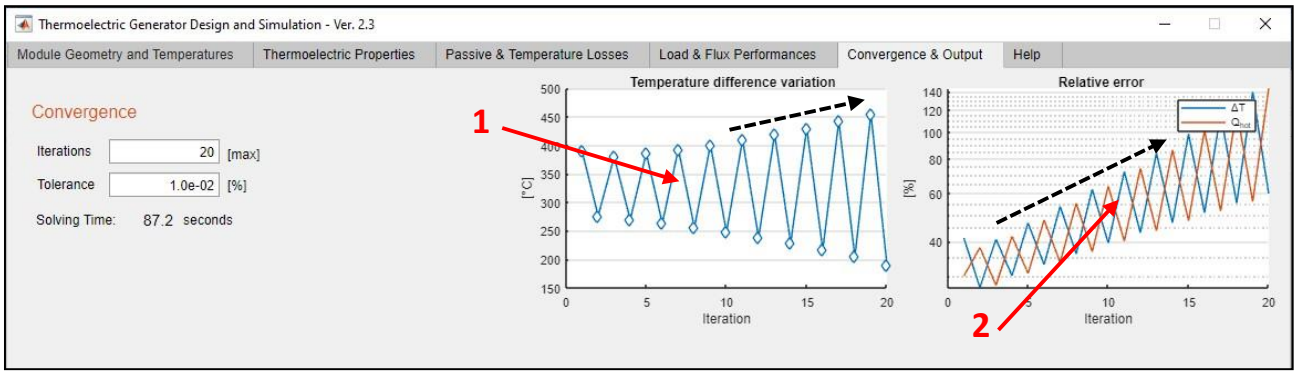
A **Warning** appears if relative error between last two value of ΔT or Q is higher than set tolerance. In this case increase the maximum number of iterations or decrease the tolerance. However, this is not critical for simulation results.



Instead, an **Error** is given if the algorithm did not converge!



This could append if the overall passive conductance is low with respect to the TE couples conductance. In this case, progressive temperature losses became too high and corrected temperature difference oscillates (1). Thus, relative error increases (2). Consider revise your geometry (e.g. higher TE elements or thinner ceramics) and material properties instead of modify number of iterations or tolerance!



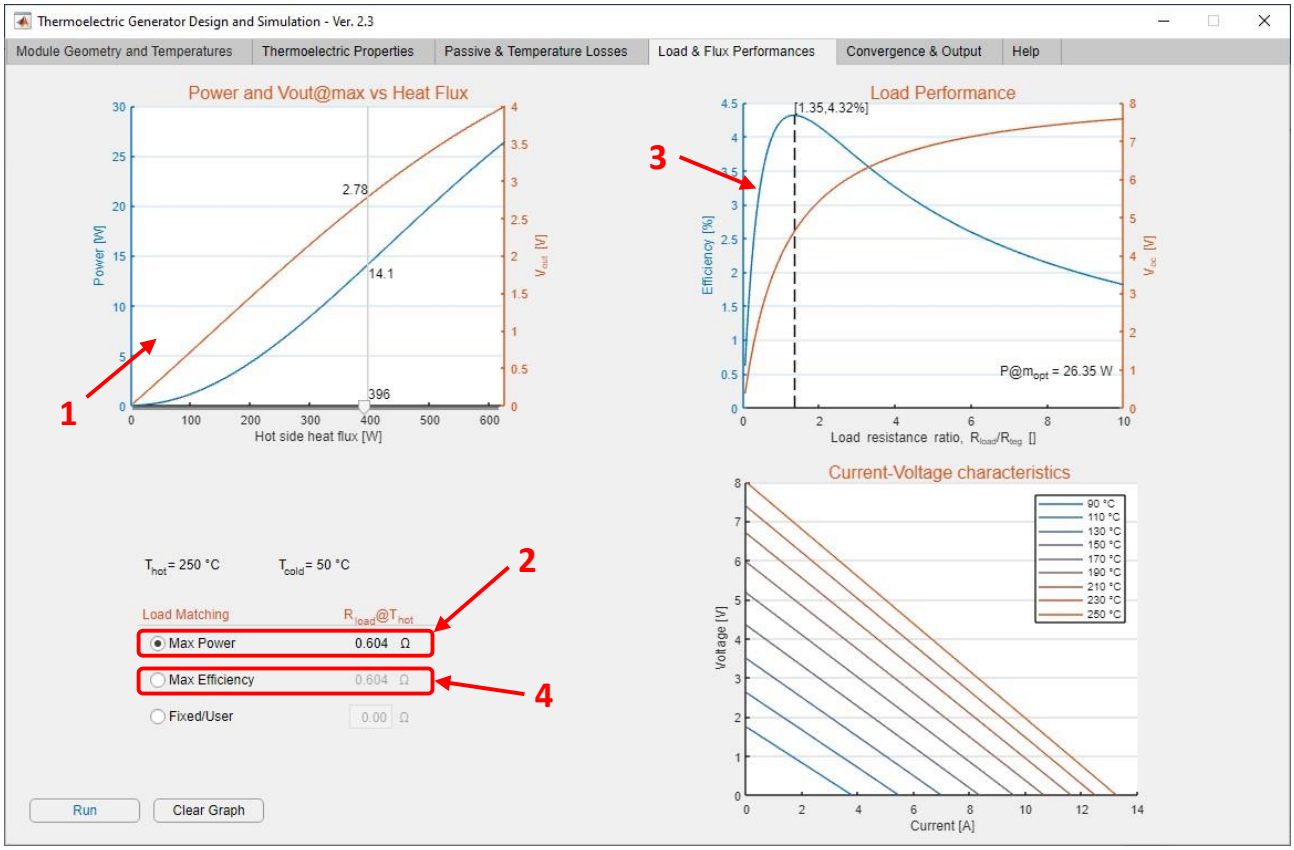
6 – Results

In **Module Geometry and Temperatures** tab main results of designed thermoelectric module are plotted. Enable the cursor and change the temperature with the slide bar to view numeric results at selected temperature.

In **Convergence & Output** page, export your result in selected folder (see Sec. 1) with preferred file format: `.txt`, `.csv`, `.xls` or `.mat`. This allows to easily retrieve, elaborate and compare different simulated geometries.

In **Passive & Temperature Losses** page, bottom-right plot, temperature drop on overall passives is shown both for hot and cold side. Left plot shows resulting effective temperature profiles at active elements (broken lines) at hot and cold side, which in turn determine thermoelectric performances.

To analyze the output power (P_{out}) and output voltage (V_{out}) as a function of hot side heat flux (Q_{hot}), select **Load & Flux Performances** tab. Left plot (1) shows the relation between hot side heat flux, power and *output voltage at matched load*.



By default, simulation is performed to achieve maximum power condition (2), i.e. matched load. Hence, at each temperature difference (ΔT), load resistance (R_{load}) is set equal to the internal resistance at this temperature difference: $R_{load}/R_{teg} = 1$;

Besides, left plot (3) displays the effects on performances (efficiency, η, an open circuit voltage, V_{oc}) of load resistance (R_{load}) variation with respect to internal resistance. A vertical line indicates the load resistance ratio at which the efficiency is maximize. **Note:** this value is typically different from $R_{load}/R_{teg} = 1$, and at this value the output power ($P@m_{opt}$) is slightly lower.

To performed the simulation with this load resistance value, choose *Max Efficiency* load matching from the menu (4). Run the program again. It is also possible to select a fixed load resistance (*Fixed/User*) adjustable by the user (this is sometimes an actual condition).

Informations

Email: alberto.ferrario@cnr.it

National Research Council of Italy - CNR
Institute of Condensed Matter Chemistry and Technologies for Energy - ICMATE
CNR - ICMATE
Corso Stati Uniti, 4
35127 - Padova IT
Ph.+390 4982958774
Mob. +39 3401480309
http://www.icmate.cnr.it