In the Excel workbook Material classification.xlsx there is an ID creation tab that tells how to assign an ID to a material. The first digit is the group, the second digit is the dimensionality of the material and the last four are the actual serial number of the material.

Each group has its own tab. Description of individual fields:

- Material id

- Short name of the material, which will be part of the name of the folder in which the properties of the material will be stored.

- Full name of the material

- Short description, if required (e.g., thin film annealed at 1000 K)

Flags are boolean values that serve to indicate in the code to which group the material belongs in terms of functionality within the heating system. A material can either be invariant, thermoelectric, a phase-change material, magnetocaloric, electrocaloric, elastocaloric or barocaloric. At the moment, these flags are mutually exclusive. Should you have a material, that is multicaloric, make two or more materials with same IDs, with different appended letters. However, if you wish to use multicaloric effect in a simulation simultaneously, open an issue and we will discuss that.

In the individual material folder there are two subfolders, appInfo and data. In the data folder, there must be descriptive files in which data sources, additional information, notes and the like are recorded in addition to the data itself. The appInfo folder contains the files we use in the TCCbuilder code. These files must always have names and contents structured in the same way (see, for example, Gd), and all data must be in basic units. These files are:

- The info.json file is in JSON format and must contain: RT properties, ranges, fields, ID, short name, long name, and melting point. The RT properties must contain the values of density, specific heat, conductivity and emissivity at room temperature. The ranges must contain the temperature ranges in which each material property is defined. Temperature ranges must be given for density, specific heat capacity, thermal conductivity, and emissivity. The fields contains strengths of the external fields where properties for caloric materials are defined. When it comes to magnetic fields, the values are in T, when it comes to electric fields, they are in MV/m, and for pressure and stress, they are in kbars. For any unknown values, input “”.

- Files rho.txt, cp.txt and k.txt (either one value at room temperature, or one column of 20000 values from 0.1 to 2000 K in steps of 0.1 K); here there are only values without temperatures.

- One or more of the above three files can be replaced by several files for different external fields (magnetic written in T, electric in MVm (which stands for MV/m), stress and pressure in kbar), e.g. cp\_0.0T.txt, cp\_1.0T.txt, etc. This happens e.g. in caloric materials.

- There are also other options where the mentioned three files are replaced by some hysteresis, e.g. cp\_heating.txt and cp\_cooling.txt, i.e. when the material’s cpThysteresis flag is true. But there can also be hysteresis with different fields, then we get cp\_0.0T\_cooling.txt, cp\_0.0T\_heating.txt, cp\_1.0T\_cooling.txt, etc. Or, we could have cp data for different values of external field without hysteresis (cpFields flag is true). Please note that the hysteresis flags tell the program which files to look for and are not necessary consistent with the actual hysteresis of the material.

- Caloric materials will have adiabatic temperature change, which must be zero outside the range, where it is defined. It must be given for the case of application of external field and removal of external field. If necessary, give information on the range of temperatures where the caloric effect is reversible in a file in data folder.