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)

The following fields are all boolean values that tell whether the data is stored in the material folder or not.

- Flags. These fields 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 implement that.

- Data on thermal properties marked in red are the properties at room temperature (~293 K) that should be available in case we do not know the temperature dependencies. These boolean values are therefore always 1 (can also be 0 if we really do not have the data).

- Other data are linked to the group within the heating system. Invariant materials, for example, have files rho(T), cp(T), k(T), but magnetocaloric materials don’t have these, because there will be separate cp(T), namely for heating and cooling at several magnetic fields (see blue colored fields). There could be even more combinations of listed properties and dependencies, and they depend on the material.

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 recorded for density, specific heat capacity, thermal conductivity, adiabatic temperature change (if the material is caloric), emissivity, and other relevant properties (e.g. seebeck coefficient for thermoelectric materials, etc.). 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 bars. (See any material for example).

- Files rho.txt, cp.txt and k.txt (either one value at room temperature, or one column of 20000 values from 0 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 means MV/m)), 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.