V Excel workbooku *Material classification.xlsx* je zavihek ID creation, ki pove, kako materialu dodelimo ID. Prva cifra je skupina, druga cifra je dimenzionalnost materiala in zadnje štiri so dejanska zaporedna številka materiala.

Vsaka skupina ima svoj zavihek. Opis posameznih polj:

* Id materiala
* Kratko ime materiala, ki bo del imena mape, v kateri bodo shranjene lastnosti materiala.
* Polno ime materiala
* Kratek opis, če je ta potreben (npr., thin film annealed at 1000 K)

Naslednja polja so vsa boolean vrednosti, ki povejo, ali je podatek shranjen v mapi materiala ali ne.

* Flags. Ta polja služijo temu, da v kodi označimo, v katero skupino material spada glede na funkcionalnost znotraj toplotnega sistema. Če je material invariant, ne more biti nič drugega. Sicer pa ima lahko več flagov.
* Podatki o toplotnih lastnostih, označeni z rdečo, morajo biti v mapi materiala vedno prisotni. To so lastnosti pri sobni temperaturi (~293 K), ki morajo biti na voljo v primeru, da ne poznamo temperaturnih odvisnosti. Te boolean vrednosti so zato vedno 1.
* Ostali podatki so vezani na skupino znotraj toplotnega sistema. Invariantni materiali bodo npr. imeli datoteke rho(T), cp(T), k(T), magnetokalorični pa rho(T), k(T), cp(T) pa ne, ker bo teh cp(T) več, in sicer za heating in cooling pri več magnetnih poljih (glej modro obarvana polja). Teh kombinacij, katere lastnosti in odvisnosti bodo navedene, je lahko še več, in so odvisne od materiala.

V mapi posameznega materiala sta dve podmapi, appInfo in data. V mapi data morajo biti opisne datoteke, v katerih so poleg podatkov zabeleženi viri podatkov, dodatne informacije, opombe in podobno. V mapi appInfo so datoteke, ki jih uporabljamo v kodi TCCbuilderja. Te datoteke morajo imeti vedno enako strukturirana imena in vsebino (glej npr. pri Gd), vsi podatki pa morajo biti v osnovnih enotah. Te datoteke so:

* Datoteka info.txt vsebuje zaporedoma ID materiala, kratko ime in temperaturo tališča, ločeno z vejicami.
* Datoteke rho.txt, cp.txt in k.txt (bodisi ena vrednost pri sobni temperaturi, bodisi en stolpec 20000 vrednosti od 0 do 2000 K v korakih po 0.1 K); tu notri so samo vrednosti brez temperatur.
* Ena ali več od zgornjih treh datotek je lahko zamenjana z več datotekami pri različnih zunanjih poljih (magnetno zapisujemo v T, električno v MVm (kar pomeni MV/m)), npr. cp\_0.0T.txt, cp\_1.0T.txt, itd. To se zgodi npr. pri kaloričnih materialih.
* Obstajajo tudi druge opcije, kjer so omenjene tri datoteke zamenjane z neko histerezo, npr. cp\_heating.txt in cp\_cooling.txt, tj. kadar ima material cpThysteresis flag true. Lahko pa je histereza tudi pri različnih poljih, takrat dobimo cp\_0.0T\_cooling.txt, cp\_0.0T\_heating.txt, cp\_1.0T\_cooling.txt itd.
* Datoteka RT properties.txt je v JSON formatu in mora vsebovati vrednosti gostote, specifične toplote, prevodnosti in emisivnosti pri sobni temperaturi.
* Datoteka Ranges.txt je v JSON formatu in mora vsebovati temperaturna območja, pri katerih je posamezna lastnost materiala definirana. Temperaturna območja morajo biti zapisana za density, specific heat capacity, thermal conductivity, adiabatic temperature change (če je material kaloričen), emissivity, in ostale relevantne lastnosti (npr. seebeckov coefficient pri termoelektričnih materialih ipd.).
* Datoteka Fields.txt vsebuje stolpec z jakostmi zunanjih polj, pri katerih so definirane lastnosti za kalorične materiale. Ko gre za magnetna polja, so vrednosti v T, ko gre za električna, so v MV/m, pri pressure in stress pa v barih.

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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. If the material is invariant, it cannot be anything else. Otherwise, it can have several flags.

- Data on thermal properties marked in red must always be present in the material folder. These are the properties at room temperature (~293 K) that must be available in case we do not know the temperature dependencies. These boolean values are therefore always 1.

- 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.txt file contains the material ID, short name and melting temperature in sequence, separated by commas.

- 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 (magnetically written in T, electrically 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 has the cpThysteresis flag 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.

- The RT properties.txt file is in JSON format and must contain the values of density, specific heat, conductivity and emissivity at room temperature.

- The Ranges.txt file is in JSON format and 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.txt file contains a column with the 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.