The European Materials Modelling Council

MODA-1

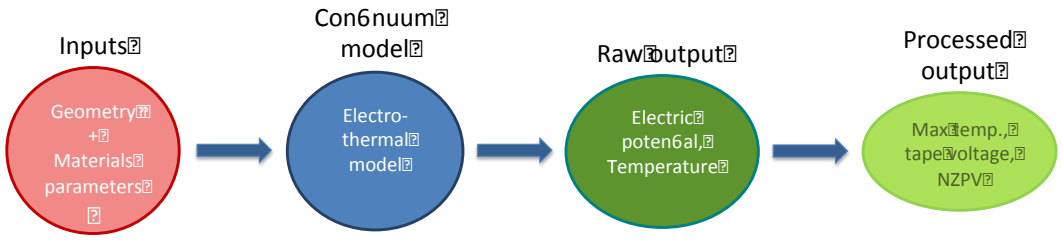
Modelling data documenting "Quench simulations in 2G HTS CCs"

FASTGRID, Quench, MODA-1

Metadata for these elements are to be elaborated over time

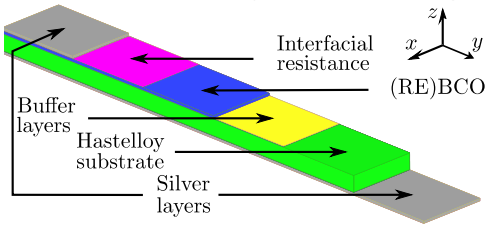
Purpose of this document:
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the computational modelling details.

OVERVIEW of the simulation			
1	USER CASE	*A figure of merit must be calculated to compare the performances of various high temperature superconductor (HTS) coated conductor (CC) tape architectures (different materials properties and geometric configurations) in which there are weaker regions where hot spots will nucleate, thus initiating a quench propagation*	
2	CHAIN OF MODELS	MODEL 1	***Fully coupled electro-thermal model.***
3	PUBLICATION ON THIS SIMULATION		
4	ACCESS CONDITIONS	*The model was developed by C. Lacroix and F. Sirois, from Ecole Polytechnique de Montreal (EPM) in the COMSOL Multiphysics commercial code. The model files are not yet publicly available. However, since EPM is one of the partners of the FASTGRID European project, there is no issue to access the model files. The participation of EPM in this project also ensures that the know-how to parameterize and execute these simulations is present in the project right from the beginning.* *Materials data required for this project are available from public literature. For the classical tape architectures, these materials properties are already included in the COMSOL model files that EPM will provide.*	
5	WORKFLOW AND ITS RATIONALE	*All desired outputs will be obtained with one simulation model, so our methodology involves a single one-step procedure (see picture below:* **Workflow of a "Quench" simulation***).* *The problem is highly nonlinear (especially the material properties), so it is simulated in the time domain. It is not possible to linearize the simulation in any way to speed it up.* *The 3-D nature of the model is also unavoidable since patterns in thin films need to be modelled and are known to have a substantial impact on the overall performance of the tape in its final application.*	



Workflow of a "Quench" simulation

Detailed documentation of a "Quench" simulation

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*The typical user case is to fix the choice of materials and geometric parameters of an HTS tape, then submit this tape to a transport current and evaluate how it responds upon the appearance of a hot spot. In output, three quantities need to be provided:* *i) the maximum temperature achieved at the hot spot (T_{max}),* *ii) the total voltage developed at the terminals of the simulated tape (V_{tape}),* *iii) the normal zone propagated velocity (NZPV)* *These outputs are the best figures of merit that allow comparing the performances of various tapes architectures, and will guide the manufacturers towards efficient solutions without losing time on approaches with little benefits.*
1.2	MATERIALS	*The materials entering in the fabrication of HTS tapes are listed in 1.3. More specifically, we have: silver and/or other metals (for the stabilizer layer), various oxides, such as CeO_2 or others (for the interfacial resistance and also for the buffer layers), (RE)BCO (for the superconducting layer) and stainless steel or nickel alloys (for the substrate). Knowing the exact chemical compositions of these materials are not so important for the continuum-type simulations that we are performing within this project: as long as we know the electrical and thermal properties of our materials, as characterized experimentally or taken from literature, this is sufficient, but their temperature dependence must be accurate.*
1.3	GEOMETRY	*The typical geometry of an HTS tape is illustrated below. Note that the silver layer (also called stabilizer) can also be present on the side edges of the tape.*  *The typical dimensions of a tape are:* *-Length: 5-100 mm (sufficient for most cases)* *-Width: 4-12 mm* *-Thickness of layers:* *-Silver: 0.1-3 um* *-Interfacial resistance: 10-100 nm* *-(RE)BCO: 1-3 um* *-Buffer layers: 0.2-1 um* *-Substrate: 50-100 um*
1.4	TIME LAPSE	*The quench process to be simulated lasts typically from 10 ms to 1 s.*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*An HTS tape used as fault current limiter is cooled down in a liquid nitrogen environment at 77 K or slightly below that (but not less than 65 K) if we work in sub-cooled conditions.*
1.6	PUBLICATION ON THIS ONE SIMULATION	

Formatiert: Deutsch (Deutschland)

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Continuum modelling of materials – Electro-thermal model*	
2.1	MODEL ENTITY	*3-D volume corresponding to an HTS tape (see picture above)*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	*Laplace equation for the electric potential:* $$\nabla \cdot (-\sigma(T)\nabla V) = 0, \quad (1)$$ *Heat equation:* $$\rho_m C_p(T)\frac{\partial T}{\partial t} + \nabla \cdot (-k(T)\nabla T) = Q_j, \quad (2)$$ *Coupling equation (Joule losses):* $$Q_j = \sigma(T)(-\nabla V)^2, \quad (3)$$ *Equations (1) and (2) are very tightly coupled through (3). The only option to achieve good convergence is to solve them simultaneously.*
		Physical quantities	*The model solves for 2 states variables, i.e.:* *i) Electric potential: V (scalar field)* *ii) Temperature: T (scalar field)* *Since the problem is 3-D, the raw output is a map of V(x,y,z,t) and T(x,y,z,t) everywhere in the simulated volume.*
2.3	MATERIALS RELATIONS	**Relation**	1. *Electrical conductivity of all materials EXCEPT (RE)BCO → sigma(T): (1,3) → Interpolation table from literature* 2. *Electrical conductivity of (RE)BCO → sigma_SC(T,E): (1,3)* $$\sigma_{sc}(T) = \frac{J_c(T)}{E_0}\left(\frac{\|E\|}{E_0}\right)^{\frac{1-n(T)}{n(T)}}$$ $$J_c(T) = \begin{cases} J_{c0}\left(\frac{T_c - T}{T_c - T_0}\right) & \text{for } T < T_c \\ 0 & \text{for } T_c \le T \end{cases}$$ $$n(T) = \begin{cases} (n_0 - 1)\left(\frac{T_c - T}{T_c - T_0}\right)^{1/4} + 1 & \text{for } T < T_c \\ 1 & \text{for } T_c \le T \end{cases}$$ 3. *Thermal conductivity of all materials → kappa(T): (2) → Interpolation table from literature* 4. *Specific heat capacity of all materials → C_p(T): (2) → Interpolation table from literature*
		Physical quantities/ descriptors for each MR	1. *Electrical conductivity of all materials EXCEPT (RE)BCO → No specific parameter since interpolation table* 2. *Electrical conductivity of (RE)BCO → sigma_SC(T,E): (1,3)* *J_{c0}: critical current density in self-field (constant)* *n_0: power-law exponent at temperature T_0* *T_c: Critical temperature* *$J_c(T)$: Critical current density as function of temperature* *n(T): Power law exponent as function of temperature* *E_0: Constant (1E-4 V/m)* *E: Electric field (E = – grad(V))* 3. *Thermal conductivity of all materials → kappa(T): (2) → No specific parameter since interpolation table* 4. *Specific heat capacity of all materials → rho_m(T): (2) → No specific parameter since interpolation table*
2.4	SIMULATED INPUT	*Not applicable: all inputs are specified by the user (geometry and materials parameters)*	

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This chapter is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	*Finite element method (nonlinear time transient simulation)*	
3.2	SOFTWARE TOOL	*COMSOL Multiphysics, available commercially, and already accessible to many of the consortium members*	
3.3	TIME STEP	*Adaptive time steps using the built-in solver of COMSOL Multiphysics (customized version of the widespread DASSL solver – used in particular in the Matlab ODE solvers suite)*	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*a) Physics equations are defined at high level in their strong form, and a finite element weak form is internally handled by COMSOL Multiphysics* *b) Materials equations are treated according to the two following cases* *i) Interpolation tables are entered directly in the front-end of the program* *ii) Analytical functions are entered as such and are evaluated as required by the low-level matrix assembly engine* *The equations apply to the entire 3-D domain being simulated, with material properties being different from domain to domain.* *Note that since we use a commercial code, we do not know exactly all the internal details, so it is difficult to describe with extreme details the numerical implementation.*
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	*Boundary conditions for V are mostly Neumann boundary conditions, meaning that the current must flow within the simulated domain. A current constraint is added to force a precise electrical current to flow in the tape (and thus one of the faces of the tape is associated to an unknown electric potential, which turns out to be a Langrage multiplier in the final system of equations.* *Boundary conditions for T are also Neumann everywhere where the tape is thermally insulated (adiabatic condition), except on the faces where cooling is present. In this case, the Newton law of Cooling can be used, with an effective convection coefficient between liquid nitrogen and the conductor face.*	
3.6	ADDITIONAL SOLVER PARAMETERS	*Relative tolerance of 0.1-1% on all state variables is usually sufficient to achieve convergence.*	

Post processing

The "raw output" calculated by the model is per definition the physics variable in the PE(s).
This is already specified in the entry 2.2 and will appear in your dark green circle in the workflow picture.

This output is often processed by a post processor in order to calculate values for physics variables for different entities that can be input to the next model. Or the output is homogenised for larger volumes in the form of a MR or Descriptor Rule that are the final output of the total simulation.
This will appear in your light green circle in the workflow picture and also in 2.4 of the next model.

The methodology (often including new physics) used to do this calculation is to be documented.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*Both raw state variables V and T are post-processed to extract the desired outputs:* *i) the maximum temperature achieved at the hot spot (T_{max}),* *ii) the total voltage developed at the terminals of the simulated tape (V_{tape}),* *iii) the normal zone propagated velocity (NZPV)*

4.2	**METHODOLOGIES**	*In the case of T_{max}, one only need to probe the evolution of temperature at the hot spot location, and find the maximum value of the field in that part of the geometry.* *In the case of V_{tape}, one just needs to take to potential difference between the surface of the tape at the tape end terminal and at the hot spot location.* *Finally, the NZPV requires more work: one must compute the speed at which the temperature T_c progress over time. Alternatively, one can also fix a voltage criterion, and see how fast this voltage propagates over time. Both approaches give the same result within 1% of accuracy.* *No output is re-used in successive simulation since our model is a single-step one.*
4.3	**MARGIN OF ERROR**	*The results are accurate within an interval of confidence that does not exceed that of the accuracy of the material models themselves. If we assume the material models as perfect, the numerical simulations agree within a few percent with the mathematical solution.*