A Discussion to Model Exothermic Reactions and Irreversible Variations of Electrical Conductivity

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Abstract

The purpose of this study is to predict, with a multiphysics model, the degradation area of a composite material when a current is injected into the material. The main physical phenomenon is an exothermic reaction, with an irreversible nonlinear variation of the electrical conductivity. The strategy is presented, in order to perform a computation that correctly takes the physics into account.

Firstly, different trials, in order to model the irreversible variation of the conductivity, are discussed: the use of a Boolean for triggering the conductivity shift, then the use of an operator in order to latch the last value of the conductivity.

Secondly, the limitation of the heat transfer with phase change material for modeling exothermic phenomena, is presented. An alternative method is presented, which allows modeling both the exothermic phenomenon, and the reaction kinetics, without the use of any mathematical tip. The reaction progress is described through a parameter $0<m(t)<1$, with an equation:

$dm/dt=-k \times m(t) \times b$, where k is the reaction kinetics and b is a Boolean when the reaction is activated.

The exothermic reaction is described by introducing a power density source:

$Q(t)=m(t) \times \Delta H \times d \times k \times b$, where ΔH is the reaction enthalpy and d is the material density.

Reaction enthalpy and reaction kinetics come from DSC (Differential Scanning Calorimetry) and TGA (Thermo-Gravimetric Analysis) measurements. Results are presented on a simplified model. An example of mapping for reaction progress m(t) and heat power density Q(t) is shown in Fig. 1 and Fig. 2 respectively.

At last, the global calculation is presented on a simplified canonical case.

Reference

[1] J. Rivenc et al., A Multiphysics Approach to Predict the Degradation of a Composite Material due to Current Injection, to be published in the Proceedings of the 17th European Conference on Composite Materials, June 27-30 (2016)

Figures used in the abstract

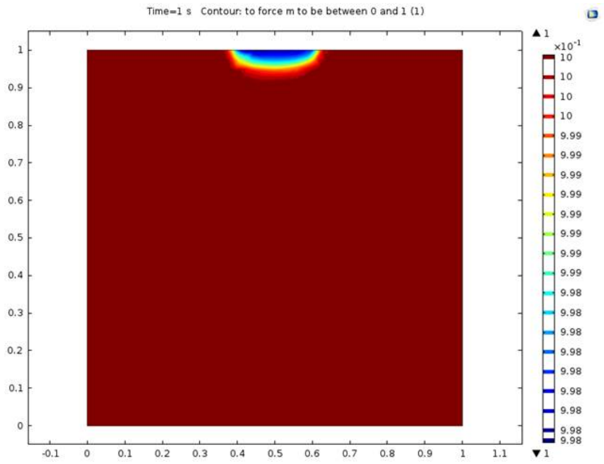

Figure 1: Mapping of reaction progress.

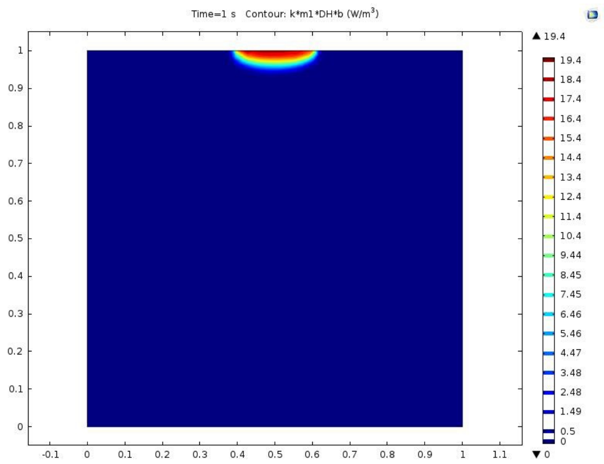

Figure 2: Mapping of heat power density.