A Novel Physics Interface for Nakamura Crystallization Kinetics

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Abstract

Prediction of crystallization is of first interest in several industrial applications (forming processes, phase change flow, energy efficiency). In the field of thermoplastic polymer forming processes, solidification is ruled by crystallization of the macromolecules [1]. Classically at the macroscopic scale, one defines a scalar variable, the degree of crystallization, which quantifies the advancement of the crystallization transformation and varies between 0 and 1. First kinetics models were based on geometrical assumptions [2]. Nakamura [3] extended these models to account for nonisothermal conditions. The Nakamura crystallization kinetics is very widely used to predict advancement of the crystallization transformation in polymer forming processes [1, 4, 5, 6, 7].
When simulating such forming processes, one needs to predict this degree of advancement at each location versus time [8, 9]. The Nakamura kinetics, in its differential form [10], states that the degree of advancement follows a local first order nonlinear ordinary time differential equation (domain ODE). Standard time integration schemes can be used to solve for this domain ODE. Nonetheless, particular numerical care has to be taken, as the right hand side (the Nakamura function) of this domain ODE presents two singular points (see Fig. 1). In this paper, a modified Nakamura function is proposed in order to overcome these singularities.
The obtained domain ODE could be implemented in any COMSOL Multiphysics® model using the domain ODE node. After having done so for several years, with multitude of models, we decided to implement this Nakamura kinetics in a novel physics node, using the Physics Builder in COMSOL. First, this enables to implement once and for all the Nakamura function modification (see Fig. 2). Then, it simplifies eventual coupling with heat transfer (exothermal computation, for instance). And finally, it eases the creation of new models by providing readily available physical material properties (see Fig. 3). In addition, all the variables now have physical names and consistent units.
Finally, as an illustration, a typical multiphysical test case is presented. A two dimensional rectangle, initially hot and molten is cooled from the right and upper edges. The model solves for the coupling between heat transfer and this novel crystallization kinetics, using the home made physics node (see Fig. 4). Material properties adapted from the literature for PEEK polymer [11] are used.

Reference

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Figures used in the abstract

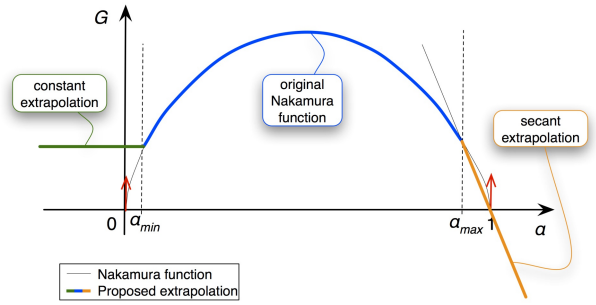

Figure 1: The original Nakamura function G is singular when \alpha=0 and when \alpha=1 (vertical tangent, materialized by the red arrows). In the proposed modified extrapolation, a thresholding is performed below \alpha_{min}, and a linear extrapolation above \alpha_{max}.

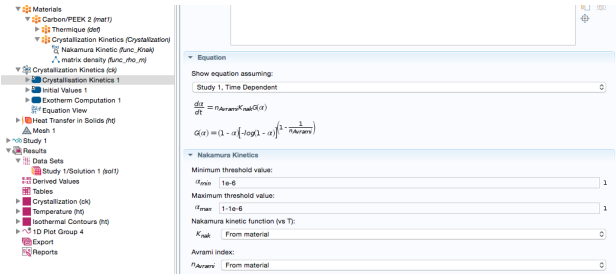

Figure 2: The new "Crystallization Kinetics" physics node is implemented once and for all using the physics builder.

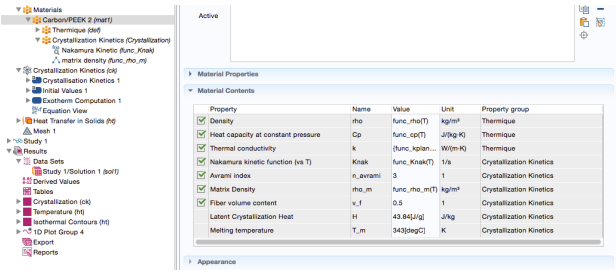

Figure 3: The new physics includes material properties consistent with the Nakamura crystallization magnitudes.

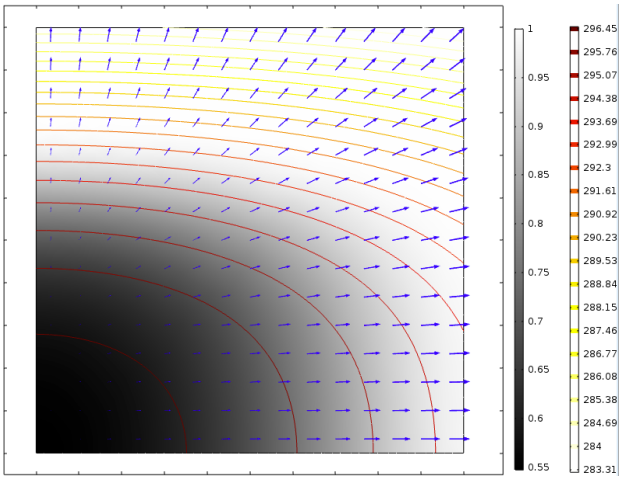

Figure 4: A typical use of the new crystallization physics is for solving a coupled heat transfer and crystallization problem in the cooling stage of polymer forming process. The surface plot represents degree of crystallization, the lines are isothermals and the arrows heat flux.