

eRAMZES – NOVEL APPROACH FOR SIMULATION OF REACTIVE MOLDING PROCESS

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KEYWORDS

Reactive molding, Computational Fluid Dynamics, Finite Element Method, Automated meshing, Web-based computations.

ABSTRACT

This paper describes a unique multiphysics simulation tool allowing one to analyze and optimize reactive molding process used for the production of electrical insulation (in the form of epoxy resin embedding) in many power products. The presented methodology differs from the standard approach, since it excludes the requirement for high end-user's knowledge and experience in the area of CFD (Computational Fluid Dynamics) and mechanical simulations. The role of the tool user is limited only to the definition of CAD geometry and process parameters via user-friendly Website. The remaining operations involved in numerical computations, including CAD geometry analysis and discretization, solving and post-processing, are executed automatically and the simulation results are published online. In this way the presented tool gives engineers an opportunity to verify the product/mold design and manufacturing process prior to the production launching or to improve the existing solutions without time-consuming and expensive experimental trials. In addition, the time needed to perform simulation (especially to prepare numerical mesh) is significantly shortened.

INTRODUCTION

Reactive molding process is an excellent area where advanced computer simulations can be utilized to design, optimize and visualize products digitally and evaluate different design concepts before incurring the cost of physical prototypes. This is a typical virtual prototyping approach (De Paolis et al. 2007) that on the one hand leads to the cost decrease and on the other hand provides useful information about highly complex phenomena taking place during reactive molding process. This, in turn, allows one to detect technological problems such as premature gelation, undesired weld-line locations, air traps or cracks (Wang et al. 1991, Macosko 1989, Grindling and Gehrig 1998) even prior to the mold manufacturing. In the traditional approach to the analysis of the reactive molding process (Sekula et al. 2000) all design

stages are executed manually by engineers utilizing different autonomous computer programs that are not directly linked to each other. These operations are time-consuming and require from the user a specialized expertise in many areas connected with numerical modeling. In the meantime, taking into consideration the industrial scale and complexity of products geometries and complicated physical phenomena taking place during the described technological process it is expected, especially by business units often located far away from Research & Development or Technical Centers, to possess an access to automated method (including generation of Finite Volume Method and Finite Element Method meshes, CFD and mechanical computations, reporting) providing high quality and reliable numerical simulations of the reactive molding process.

As a consequence, a new Web-based and automated tool linking several state of the art numerical software, called eRAMZES, has been developed to give engineers, even not familiarized with computer-aided-engineering problems, an online and, hence, unlimited access to advanced reactive molding simulations (Rajca et al. 2010a, Rajca et al. 2010b, Rajca et al. 2011). This opened totally new horizons for the analysis and optimization of the products manufactured in reactive molding technology.

BASIC PRINCIPLES OF THE REACTIVE MOLDING PROCESS

The mentioned automated simulation tool is dedicated to the analysis of products manufactured in APG (Automated Pressure Gelation) process, which is one of the leading reactive molding technologies (Sekula et al. 2003). In this process, which is presented schematically in Figure 1, two or more liquid reactants with additional components are mixed in the first step. Then, after homogenization and degassing, the mixture is introduced by injection system into the heated mold (filling stage). Polymerization of the resinous material (curing stage) results in its phase change from the liquid form to the solid body (final product shape). Afterwards, de-molding stage occurs and product is placed most often in a tunnel furnace (Ashmad et al. 2006) (post-curing stage) in order to finish the curing process and finally to release thermal and chemical stresses applying gradual product cooling.

MATHEMATICAL MODELING OF THE REACTIVE MOLDING PROCESS

The complexity of the reactive molding process is presented in Figure 2 illustrating different phenomena taking place during all stages involved in APG technology, i.e. filling, curing and post-curing. Each phenomenon is reflected in an appropriate mathematical model implemented in the developed simulation tool. In the case of CFD analysis (run in a commercial CFD software ANSYS FLUENT) one have to deal not only with numerically unstable multiphase flow calculations, but also with the kinetics of curing reaction and conjugate heat transfer. Additionally, because of the dynamics of the chemical reaction and complexity of the resulting thermal effect, an accurate modeling of the stresses and deformations during mechanical analysis (run by using another commercial application dedicated to structural analyses, i.e. ABAQUS) is not an easy task.

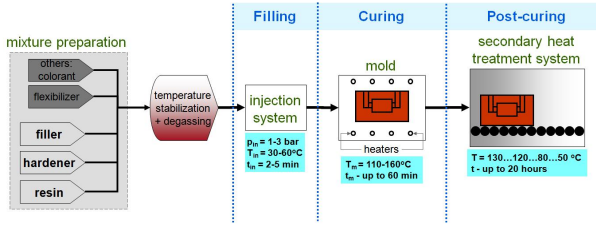


Figure 1: Scheme of the reactive molding process

One can find in the following part of this paper a brief description of models used in fluid mechanics, thermal and mechanical calculations offered by the presented tool as well as in materials characterization (Sekula et al. 2003).

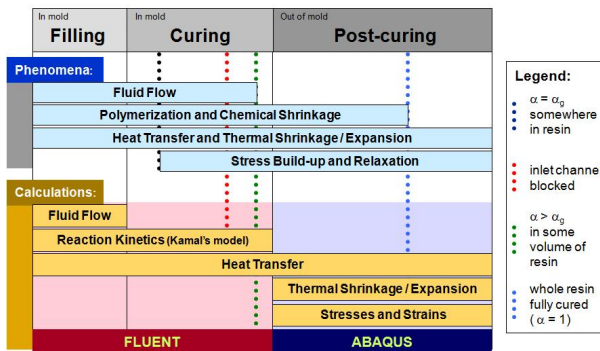


Figure 2: Complex nature of the APG process

CFD simulations

Because of the principle of the conservation of material the solution must satisfy the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

where t is time, ρ is density and u velocity of the fluid. From Newton's second law one can obtain the dynamical equation describing the fluid motion, namely the momentum equation:

$$\rho \frac{Du}{Dt} = \nabla \cdot (\tau) - \nabla p - \rho g \quad (2)$$

where p is pressure, τ is the stress tensor (whose components are the function of viscosity η and spatial derivatives of u), g is acceleration due to the gravity and Du/Dt term is the substantial (or particle) derivative of the velocity computed by following a particle in the flowing substance.

Due to the presence of two different fluids during the mold filling stage (epoxy resin and air) volume of fluid method (VOF) is used to predict accurately the location of the interface between both phases. In the VOF approach the volume fraction of the resin a in each cell is solved from the conservation equation:

$$\frac{\partial a}{\partial t} + \nabla \cdot (au) = 0 \quad (3)$$

where $a = 0$ means no epoxy resin in the cell, $0 < a < 1$ means partly filled cell, $a = 1$ means cell filled totally with epoxy resin and the volume fraction of air b is the complement of a (i.e. $b = 1-a$).

The nature of the reactive molding process causes that it is important to monitor the course of polymerization reaction of thermosetting epoxy resin. For this purpose curing kinetics model in the form of Kamal-Sourour equation is applied (Kamal and Sourour 1973, Kamal et al. 1973) and implemented in ANSYS FLUENT by using User Defined Function and User Defined Scalar functionalities (ANSYS Help 2010). According to this model degree of curing α at time t is defined as:

$$\alpha = \frac{H(t)}{H_{\Sigma}} \quad (4)$$

where $H(t)$ is the heat of reaction released until time t and H_{Σ} is the total heat of reaction.

The progress of the curing phenomenon is linked to the mass conservation and thus the degree of curing α is governed by its own un-steady state conservation equation:

$$\frac{\partial(\rho\alpha)}{\partial t} + \nabla \cdot (\rho u \alpha) = S_a \quad (5)$$

where S_a is the source term of degree of curing based on the mentioned Kamal-Sourour model expressed by the equation below:

$$S_a = \rho(k_1 + k_2\alpha^m)(1-\alpha)^n \quad (6)$$

where m and n are the model constants, whereas k_1 and k_2 are the reaction rate constants calculated as follows:

$$k_i = A_i e^{\left(\frac{-E_i}{RT}\right)} \quad (7)$$

where $i = 1$ or 2 , A_i is the pre-exponential factor, E_i is the activation energy, R is the universal gas constant and T is the absolute temperature. It is worth stressing that all parameters of Kamal-Sourour model are determined experimentally, usually by using Differential Scanning Calorimetric technique, and their values are characteristic for each epoxy resin. Conservation of energy is guaranteed by the energy equation in the form:

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T \right) = \nabla \cdot (k \nabla T) - \rho \nabla \cdot u + \nabla \cdot (\tau \cdot u) + S_T \quad (8)$$

where c_p is the specific heat capacity, k is the thermal conductivity and the source term of thermal energy is calculated as $S_T = S_a H_\Sigma$.

Data transfer between CFD and mechanical stage

As soon as the CFD calculations are completed, the results (temperature and degree of curing) have to be transferred from CFD mesh (Finite Volume Method) into structural mesh (Finite Element Method) for mechanical calculations. Since no adequate direct data transfer codes are available on the market, an external data transfer procedure called MapMesh was developed in the course of this study and successfully implemented to perform the solution mapping between CFD and structural numerical models. More detailed description of the CFD simulation approach and the data transfer mechanism is provided in [Isotalo et al. 2001](#).

Mechanical simulations

The structural results are obtained in a transient and coupled thermal and stress analyses conducted sequentially as presented in Figure 3. In the first step the effects related to the heat transfer are determined and then chemically driven deformations are calculated in the static analysis. Finally, this leads to the definition of the strains and stresses as a function of the process time.

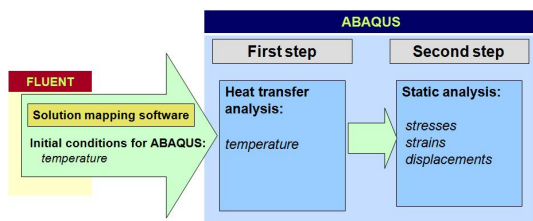


Figure 3: Sequential calculations in ANSYS FLUENT and ABAQUS

The chemical shrinkage model was developed based on the assumption that the total strain increment $\Delta \varepsilon^{\text{Total}}$ (in each time-step) can be expressed as a sum of mechanical $\Delta \varepsilon^{\text{Mechanical}}$ and thermal $\Delta \varepsilon^{\text{Thermal}}$ components:

$$\Delta \varepsilon^{\text{Total}} = \Delta \varepsilon^{\text{Mechanical}} + \Delta \varepsilon^{\text{Thermal}} \quad (9)$$

ABAQUS software allows defining thermal component by applying a user-defined subroutine (UEXPAN). This component covers both chemical and thermal effects influencing the material density:

$$\Delta \varepsilon^{\text{Thermal}} = \sqrt[3]{\frac{\rho}{\rho'}} - 1 \quad (10)$$

where ρ' means actual density and ρ is the value of density from the previous time-step. It is worth stressing that in order to realize that stage of calculations it was necessary to apply the dependence of temperature and degree of curing on density. This correlation was derived based on the experimental measurements. More information about the modeling of epoxy resin shrinkage can be found in [Isotalo et al. 2004](#).

WEB-BASED TOOL FOR AUTOMATED REACTIVE MOLDING SIMULATIONS

The architecture of eRAMZES tool

eRAMZES tool is controlled by a dedicated multifunctional Web platform linking a number of applications interacting between each other. Among them one can find software available on commercial conditions (CAD software, pre-processors, processors and post-processors) and developed specially for the purpose of simulations automation, which are fully customizable.

The general workflow of eRAMZES tool is presented schematically in Figure 4. Green boxes illustrate steps that require interaction with user, while violet boxes indicate fully automated operation of the tool. One can notice that engineer is obliged only to define the geometrical model and planned process parameters, while the remaining computational steps are executed in an automated manner. When the simulation finishes and results are visualized, the user decides whether the analyzed product and process fulfills requirements or further optimization is needed. In this way the developed approach allows engineers to design reactively molded products in an automated way by using advanced CFD and mechanical methods without expert's knowledge related to numerical modeling.

The automation applied in the presented tool is based on the concept of developed Watcher and Launcher programs. In general, Watcher software observes the progress of each task executed by the tool by analyzing the task status ('ready to start', 'work in progress' or 'finished') and controls the availability ('busy' or 'free to run' status) and operation of Launchers performing three specific tasks, namely:

- 'Pre' – preparation of the starting directory for the specific program (e.g. pre-processor or solver) maintained by a given Launcher;
- 'Launch' – launching the program;
- 'Post' – cleanup and file management after termination of the program operation.

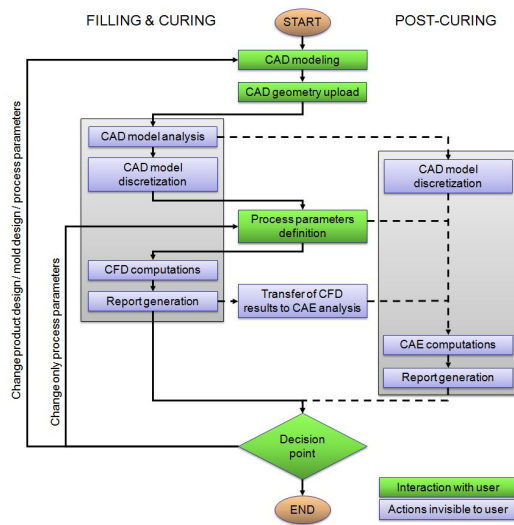


Figure 4: Architecture of the presented approach

CAD modeling

The very first step of the analysis that must be taken by user is CAD modeling, preferably in advanced CAD system like for example SolidWorks. This is a crucial operation, since engineer decides at this stage about the geometrical components, their features and possible simplifications, which will be taken into consideration during computations. Due to a big significance of this analysis step several recommendations have been worked out to guide users in the preparation of geometrical models. This concerns among others proper labeling of the geometrical parts, since only regions starting with "fluid" or "solid" prefixes are included in further simulation steps (e.g. fluid_cavity, solid_mold, solid_insert_steel etc.). In addition to that, all regions must be represented as solid bodies without Boolean operations performed on them (see Figure 5), geometry should be properly positioned in Cartesian coordinate system (e.g. symmetry plane along YZ plane for $X = 0$) and the prepared model has to be exported to STEP file.

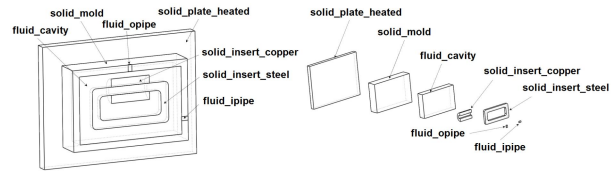


Figure 5: Proper labeling (left) and structure (right) of geometrical parts

Case creation

In the consecutive step the simulation case must be created by user via the mentioned Web platform as presented in Figure 6. This requires connection and login to the eRAMZES Website, choice of the file with the CAD geometry prepared in the previous step and activation (if applicable) of the model symmetry option and mechanical calculations.

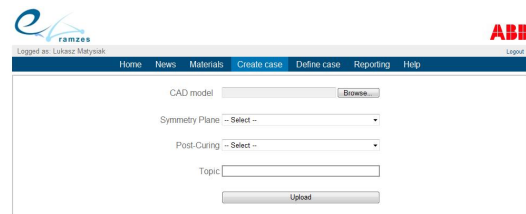


Figure 6: Case creation Web page

CAD model analysis

The uploaded CAD geometry is then analyzed automatically to detect parts included in the model and marked by user with "fluid" and "solid" prefixes at the CAD modeling stage. CAD model analysis is extremely important, because the gathered data is used further during the meshing and solving operations. Additionally, based on these information an individual Website is generated to allow user to enter the process parameters.

Numerical model preparation

Geometry discretization is the next fully automated step executed by eRAMZES, however it should be stressed that this stage was recognized as the most challenging part of the tool development, mainly due to high complexity and variety of the geometries of products manufactured in the reactive molding technology. Additionally, the mentioned differences in CFD and mechanical calculations made it necessary to perform the meshing operations in different meshing software, i.e. HyperMesh and ABAQUS for CFD and mechanical module respectively.

In the proposed approach, the mentioned Launchers initiate and control the discretization procedure in each of the mentioned pre-processors. The process

automation is ensured by scripts including a sequence of commands. In this way specific orders are given to the meshing software like import CAD geometry, clean and repair geometry (removal of holes, fillets, intersections, overlapping surfaces, etc.), discretize geometry (different mesh topologies can be used and consequently either non-structural or structural mesh can be generated), define CFD (e.g. inlet, outlet, convection etc.) and mechanical (e.g. constraints, interactions etc.) boundary conditions, export output file in CAS and INP formats for ANSYS FLUENT and ABAQUS solvers respectively.

One can find below two exemplary geometries of medium-voltage products that were analyzed by using eRAMZES tool. Figure 7 depicts the geometrical model of outdoor embedded pole and the CFD mesh generated, while Figure 8 illustrates the geometrical model of current transformer and the mechanical mesh prepared. It can be seen that high quality mesh was created automatically in both cases in spite of the complexity of components included in both geometries. An additional and simultaneously one of the biggest benefits coming with the meshing automation is the time needed to generate numerical grids. eRAMZES tool spent only 30 minutes to decompose the current transformer geometry into almost 3 million of CFD mesh elements and 300 thousand of mechanical mesh elements (by using PC computer equipped with two 2.5 GHz dual-core CPUs and 8 GB RAM), while it takes usually days or sometimes even weeks for CAE engineers to generate manually the numerical mesh for such complex geometries. This allows eRAMZES users to focus on solving engineering problems rather than spending time on models discretization.

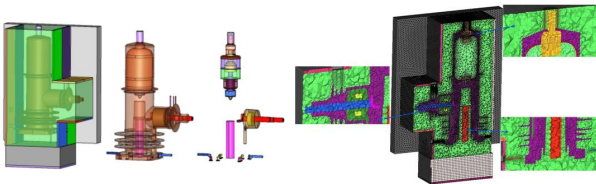


Figure 7: Geometry of outdoor pole (left) and its discretization in HyperMesh (right)



Figure 8: Geometry of current transformer (left) and its discretization in ABAQUS (right)

Process parameters definition

Definition of the process parameters is another step of the reactive molding analysis with the eRAMZES tool that requires input from the user side. The Web application uses information gathered during the CAD model analysis and creates dynamically a dedicated Website (as shown in Figure 9) allowing user to enter all parameters required to configure the simulation. At this stage both the process parameters, material properties, materials assignment to product parts and finally, numerical parameters related to mechanical computations are selected. Among the process parameters one can find injection parameters (e.g. filling time or injection velocity), thermal parameters (e.g. temperature of injected material, temperature of heaters, initial temperatures before injection), ambient conditions (e.g. air temperature or air convection intensity), post-curing procedure (time and temperature of each cooling stage). All these settings are saved by the tool in the case folder and the automated computations can be started.

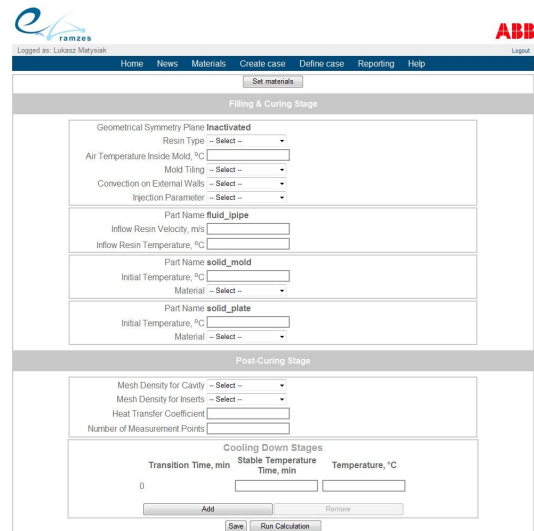


Figure 9: Definition of the process parameters

Computations

Processing (or solving) is the subsequent fully automated stage of the simulation process, executed by using scripts generated automatically and individually for each simulation case. Processors controlled again by Launchers operate in a batch mode to shorten the computational time remaining one of the critical issues reported by users.

At the very beginning of the solving step the discretized geometry is imported into the CFD processor – ANSYS FLUENT. Next, information provided by user during CAD modeling stage and process parameters definition are assigned to the numerical model to specify material for each geometrical component and to define initial conditions, boundary conditions, operating conditions and materials properties. Additionally, the solver

configuration is performed including the choice of mathematical models used in the reactive molding simulation (both built-in models like e.g. turbulence model, flow model etc. as well as additionally implemented models like curing kinetics model) and numerical parameters to ensure reliable and accurate solution of these models. In the consecutive step the transient numerical computations for filling and curing stage are conducted and, once done, results are generated and exported.

The computations can be continued if user decided to include post-curing simulation. In such case temperature results obtained for the end of curing stage are translated by using the mentioned MapMesh software and transferred to the mechanical solver ABAQUS to constitute the starting point for post-curing computations.

The first step taken by ABAQUS software is the geometrical model import and repair (if needed). Next, material properties are assigned to the geometrical parts and the analysis steps and time are specified according to the user input provided during CAD modeling and process parameters definition. In the subsequent stage boundary conditions (the mentioned data from ANSYS FLUENT, constrains, etc.) and interactions between geometrical parts are set and the mesh is generated based on the information about the mesh density specified earlier by user. Finally, the input file is prepared and submitted to solver for computations and, once finished, results are generated and exported.

It is worth noticing that the solution convergence is monitored and controlled automatically, what was recognized as one of the biggest challenges during the tool development and became one of the most significant achievements. The reason for this is that the reactive molding simulation is known as numerically instable, even in case of manual approach, due to the complexity of phenomena involved in the process. In the meantime, eRAMZES ensures excellent solution stability without any user actions.

Results visualization

Post-processing is the last step of the automated reactive molding analysis with eRAMZES tool. The simulation results are further processed in a batch-mode in ANSYS CFD-Post and built-in ABAQUS post-processor controlled by Launchers. For this purpose master macros, recorded for each post-processor individually, are executed for each simulation case making the results visualization process automated and repeatable irrespective of the product under consideration.

In the next step, the obtained results are presented to user in different forms like movies, pictures and charts via the Website or as a printable PDF document. It is worth stressing that the way of results visualization can

be modified to meet the user expectations, what constitutes another advantage of the presented approach. Exemplary results generated for CFD and mechanical analysis are presented in Figure 10 and Figure 11 respectively.

The developed way of results visualization allows users to observe in details the course of the reactive molding process and capture effects inside the mold and product, which cannot be detected in a normal production process or in an experimental way. This includes information about the flow pattern of epoxy resin during the filling stage, distribution of temperature in time during all process stages, distribution of degree of curing in time during the filling and the curing stage, distribution of deformations, stresses and strains during the post-curing stage.

The acquired knowledge is then used by engineer to decide whether further process and product optimization is needed or not. In the first case two options are possible, namely modification of the process parameters for the same product and mold geometry (CAD model upload, analysis and discretization is not repeated) or redesign of the product and/or mold (analysis process starts from the very beginning).

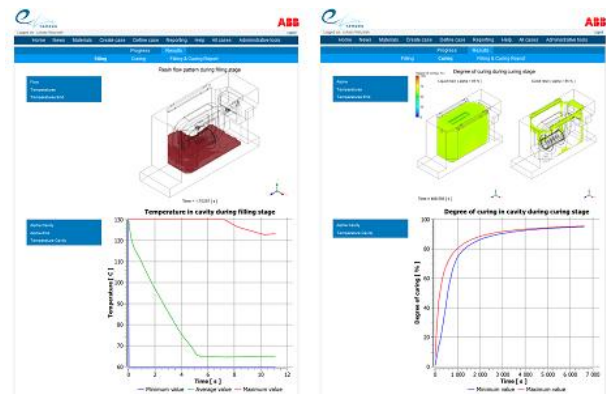


Figure 10: Results generated for filling stage (left) and curing stage (right)

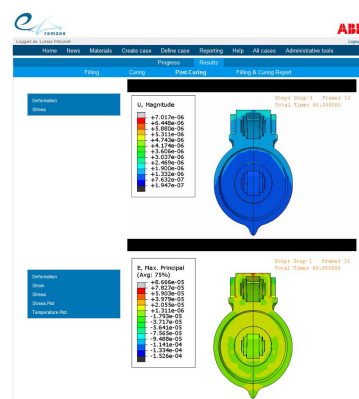


Figure 11: Results generated for post-curing stage

SUMMARY

The presented novel Web-based tool combining CFD and mechanical simulations can be successfully utilized both for the design of new and optimization of the existing products manufactured in the reactive molding technology. The tool allows users to observe the influence of changes in the product and/or mold design as well as in the configuration of the process parameters without any interference in the real production process. This was achieved by high quality simulation results presenting details about the process course.

The described automation of meshing and solving operations executed during CFD and mechanical computations allowed one to shorten significantly the total computational time and eliminate the requirement for high user knowledge and experience in the field of numerical simulations. Among the other tool advantages one can notice its user-friendliness, unlimited online access to the tool and the repeatability of the simulation process resulting in manual-error resistance.

All aspects mentioned above lead, on the one hand, to shorter development time of new products manufactured in the reactive molding technology and, on the second hand, to improved quality of the epoxy based components. Moreover, the presented approach can be adapted to provide the possibility to analyze also other manufacturing processes and, consequently, benefit in faster development and optimization of much wider group of power products, not only limited to reactively molded ones.

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