A Novel Simulation Approach for Analyzing Reactive Molding Process

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Abstract—Reactive molding process of thermosetting materials is an area where advanced computer simulations can provide useful information to detect molding problems prior to the mold making. Examples of such problems are premature gelation, undesired weld-line locations and air traps. This paper introduces newly developed simulation approach for analyzing reactive molding processes: filling and curing. The presented methodology differs from the currently used one because does not require deep end-user's CFD (Computational Fluid Dynamics) knowledge. It was possible thanks to automation of a number of typical in numerical approach stages including: CAD geometry discretization, solving and post-processing.

The presented method starts with CAD geometry preparation in accordance with the set of specific rules. In the next step the geometry is uploaded via the Website. The Web application analyzes the geometry and detects its structure in automated way. These initial information allow creating an individual Website where, in consequence, engineer (end-user responsible for the final process and product design) is able to enter process parameters (e.g. material properties, initial temperatures, velocities, etc.) and start calculations. The discretization (or meshing) and solving stages are performed in fully automated way. Finally the Web application creates the report with useful information helping to understand the phenomena occurring inside the mold. This report is also available via developed Website. Based on these information the engineer makes a decision to accept the design and process parameters or to restart the simulation for further optimization.

The presented approach helps to save time required for designing proper product and its mold. It influences directly on one of the most important global market factor means time-to-market and in the same increase product quality.

Keywords—Reactive molding, CFD simulation, automated meshing, Web-based computations

I. INTRODUCTION

THE fast development of new numerical computing techniques and availability of highly powerful working stations make it possible to reduce the time necessary to design and manufacture final products, at the same time maintaining their high quality and reliability [1]. Continuing this trend, numerical computing is more and more often used for solving design tasks on an industrial scale, where frequently in the course of implementation of methods and systems of automated product designing the designers analyze at the same time the flows of fluids and the problems of transport of heat and mass within a designed geometrical model of a product and its mold. In the case of a process in the reactive molding technology, in order to better understand the physical phenomena the knowledge of the structure of very complex 3-dimentional geometries and the ability to analyze them is required. Partial differential equations, for example Navier-Stokes equations, which describe mathematically and completely fluid movement and heat exchange, usually are not suitable for an analytic solution, with the exception of simple cases, because their degree of complication is too great. Therefore, solution of such equations on an industrial scale is possible only in a numerical way using the methods of numerical fluid mechanics.

Reactive molding is a technology widely used in processing of epoxy resins, and consists of a number of process stages, including mold filling, curing with exothermic reaction, and post-curing. This process of thermosetting materials is a very good example of industrial 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 process [2] that leads, on the one hand, to cost decrease and on the other hand can provide useful information about highly complex phenomena taking place inside the mold during the filling and curing stages and in addition to detect molding problems prior to the mold making, such as premature gelation, undesired weld-line locations and air traps [3,4,5].

Engineers today are using 3D computer-aided design/engineering/manufacturing tools to deliver many of the world's most innovative products [6]. However the existing methods and solutions are limited to numerically advanced engineers and scientists. Besides, activities that consist of CAD geometry preparation and/or simplification, computational domains discretization and finally solving are time-consuming.

Additionally nowadays we are facing fast growing market competitiveness. Time-to-market factor is the one of the most important and may influence the final product success in the global market. Therefore development time of new concepts and products must be as short as possible.

In currently used solutions [7], all the required design stages are executed manually by means of autonomous computer programs which are not directly linked to one another. Their

operation is time-consuming and requires the user to possess specialized expertise in many areas connected with numerical modeling.

That is why it was necessary to develop the new tool allowing, engineers even not familiarized with CAE problems, running advanced reactive molding simulations.

II. REACTIVE MOLDING AND MODELING PRINCIPLES

A. Reactive molding

Reactive molding technologies can be divided into two main groups:

• Vacuum casting
• Automated Pressure Gelation (APG)

Vacuum process is mainly used for large parts for high voltage applications. Usually, these products are cast in short production series and have long casting cycles (large distribution transformers coils, instrument transformers and gas insulated switch gears).

The Automated Pressure Gelation process is used for products manufactured in mass production. This process can be characterized by short molding cycles (minutes versus hours for vacuum casting) and high accuracy.

In the typical reactive molding – APG process, see Fig. 1, two or more liquid reactants with additional components are mixed. After homogenizing and degassing, the mixture is introduced by injection system, into the heated mold. Polymerization of the resinous material generates additional heat and the component becomes harder obtaining a desired shape. Afterwards, de-molding is done and secondary heat treatment, aiming curing completion is carried out - very often in tunnel furnace [6].
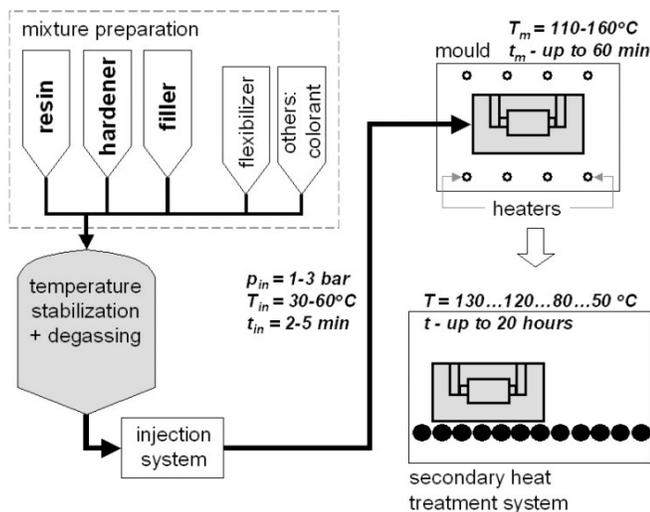
Fig. 1 Scheme of the reactive molding process [8]

B. Calculation approach – CFD procedure

The picture given below - Fig. 2 describes the phenomena taking place in three stages (filling, post-filling, post-curing) of APG process. In addition, information concerning calculations

performed is noted and it includes fluid flow calculations with viscosity model, reaction kinetics modeling, thermal and chemical shrinkage, stress and strain modeling.
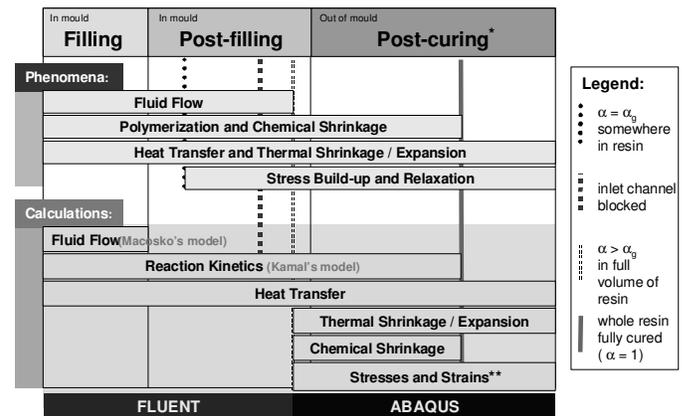
Fig. 2 Complex nature of the APG process

The proposed and implemented simulation procedure [6] involves commercial CFD software Fluent, however to calculate the behavior of thermosetting mixture two additional models were implemented (as so called user defined subroutines) in the software: Kamal's model for reaction kinetics and Macosko's model to describe the viscosity changes. In most of industrial cases the Macosko's model can be neglected when results are still accepted.

The fundamentals of the used methods for thermo- and fluid dynamic modeling and material characterizations are briefly described below [3].

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \overline{u} \right) = 0 \qquad (1)$$

Where t is time, ρ is density and $\overline{u}$ velocity of the fluid. For simplicity, we assume in this paper that each phase (i.e. resin and air) is incompressible, but in the filling stage the average density of mixture in cells containing both phases changes and that is why for generality $d\rho/dt \neq 0$ in (1).

From Newton's second law we can obtain the dynamical equation describing the fluid motion, namely the momentum equation:

$$\rho \frac{D\overline{u}}{Dt} = \nabla \cdot \left(\overline{\overline{\tau}} \right) - \nabla p - \rho \overline{g} \qquad (2)$$

where p is the pressure, $\overline{\overline{\tau}}$ is the stress tensor (these components are function of the viscosity η and the spatial derivatives of $\overline{u}$) and $\overline{g}$ is the acceleration due to the gravity. $\frac{D\overline{u}}{Dt}$ -term is the substantial (or particle) derivative of the velocity computed.

The viscosity of thermosetting material is a complex function of the shear rate $\dot{\gamma}$, the temperature T, and the extent of reaction α. The reaction extension so called conversion or

curing ratio and, as the progress of the reaction is directly linked to the curing of a thermoset, thus α can be interpreted as the degree of cure.

In many applications to obtain better accuracy the following model derived by Macosko [4] is being used:

$$\eta(\dot{\gamma}, T, \alpha) = \eta_c(\dot{\gamma}, T) \cdot f(\alpha) \tag{3}$$

where:

$$f(\alpha) = \left(\frac{\alpha_{gel}}{\alpha_{gel} - \alpha}\right)^{C_1 + C_2 \alpha} \tag{4}$$

$$\eta_c = \frac{\eta_0}{1 + C(\eta_0 \dot{\gamma})^{1-n}} \tag{5}$$

with:

$$\eta_0 = Be^{\frac{T_b}{T}} \tag{6}$$

In the equations above, η_c and η_0 present the modified cross model and the zero-shear-rate viscosity, respectively. In addition, B, T_b, C_1, C_2, C and α_{gel} (the value of α when gelation occurs) are material dependent constants. A typical value of α_{gel} is in the range of 0.65-0.75. Mostly in the current studies, the model without shear thinning effects is being applied (the power law coefficient n is set equal to 1 in equation (5)). Thus, the viscosity becomes a function of the temperature and degree of cure only.

The most important remains to determine kinetics of the curing process. In such cases the Kamal's model is used [10,11]. According to this model a degree of curing at time t is defined as:

$$\alpha = \frac{H(t)}{H_\Sigma} \tag{7}$$

where:
H(t) -heat of reaction released at time t,
H_Σ - 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:

$$\frac{\partial(\rho\alpha)}{\partial t} + \nabla \cdot (\rho\bar{u}\alpha) = S_a \tag{8}$$

where S_a is the source term of degree of curing based on the used curing kinetics model. Based on used Kamal's curing kinetics model such that

$$S_a = \rho(k_1 + k_2\alpha^m)(1-\alpha)^n \tag{9}$$

where the reaction rate constants is given as the following:

$$k_i = A_i e\left(\frac{-E_i}{RT}\right) \tag{10}$$

and:

i = 1,2;
m, n - constants,
k_i - reaction rate constants,
A_i - pre-exponential factors,
E_i - activation energies,
R - the universal gas constant,
T - absolute temperature

Conservation of energy is guaranteed by the energy equation in the form:

$$\rho c_p\left(\frac{\partial T}{\partial t} + \bar{u} \cdot \nabla T\right) = \nabla \cdot (k\nabla T) - p\nabla \cdot \bar{u} + \nabla \cdot \left(\bar{\bar{\tau}} \cdot \bar{u}\right) + S_T \tag{11}$$

where c_p is the specific heat, k is the thermal conductivity. The left-hand side of the equation (4) describes the change in the internal thermal energy including convection. The terms on the right-hand side represents – in the respective order - the heat transfer by conduction, the reversible conversion between kinetic and thermal energy, the irreversible conversion of kinetic to thermal energy due to viscous effects (i.e. viscous dissipation) and the source term of the thermal energy such that $S_T = S_a H_\Sigma$.

In the applied approach no diffusion term for the Kamal's equation was used.

Usually differential scanning calorimetry (DSC) is being employed to characterize the curing kinetics parameters. As an example sets of the resulting parameter of the curing kinetics model for the epoxy resin are summarized in Fig. 3.

PARAMETERS FOR CURING KINETICS MODEL (KAMAL)

Symbol	Value	Unit
H_Σ	103340	J/kg
A_1	2.293×10^9	1/s
A_2	1.163×10^5	1/s
E_1/R	11654	K
E_2/R	7182	K
m	0.438	-
n	1.118	-

Fig. 3 Example of the set of parameters for curing kinetics calculations [9]

Taking into consideration industrial scale of geometries and in consequence their complexity and in addition complex physical phenomena taking place during the described technology 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 for good quality numerical simulations of reactive molding processes (CFD mesh generation, CFD computations, reporting).

III. TOOL ARCHITECTURE AND DESCRIPTION

The developed tool is based on the Web platform (a number of interacting, developed program applications), commercial CAD software, commercial Pre-processor and Processor (both customizable).
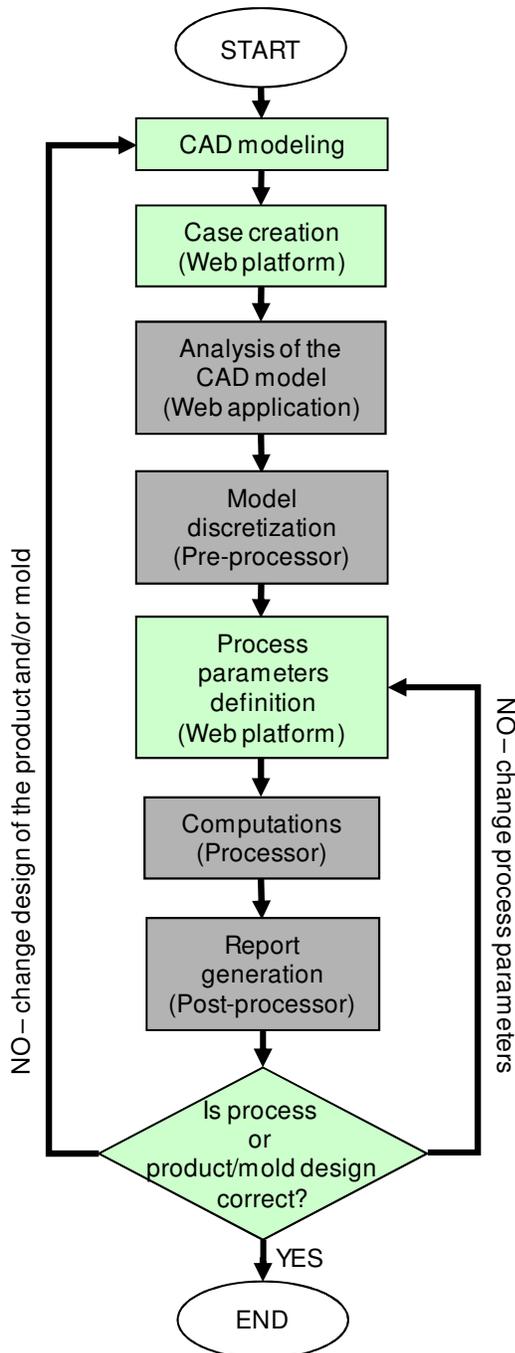
Fig. 4 Architecture of the Web-based tool

The scheme Fig. 4 we present the simplified tool architecture. In general boxes green marked mean that the end-user interactions are desired and the grey ones represent fully automated stages. Following mentioned stages allows designing reactively molded products and molds in automated way with utilizing advanced CFD solutions.

A. CAD modeling principles

The very first step is CAD modeling – geometry preparation. It is suggested to perform it in the advanced CAD software e.g. SolidWorks. During that stage it is obligatory to take several recommended actions:

• all important, from geometry and technology point of view, regions must be labeled according to the following rules:
  o all fluid and solid regions must be labeled starting with "fluid" and "solid" respectively (e.g. fluid_cavity, fluid_inlet_pipe, solid_insert_steel, solid_insert_copper, etc.), as it shown in Fig. 5a;
  o all remaining regions like for example screws, washers, wires etc. may stay unnamed but then all of them will not be taken into consideration during pre- and consequently post-processing;
• all regions must be kept as full solids (no Boolean operations on the geometry allowed), see Fig. 5b;
• the geometry symmetry should be set (if exists) on z plane (in Cartesian coordinate system);
• export the geometry to the step file format.
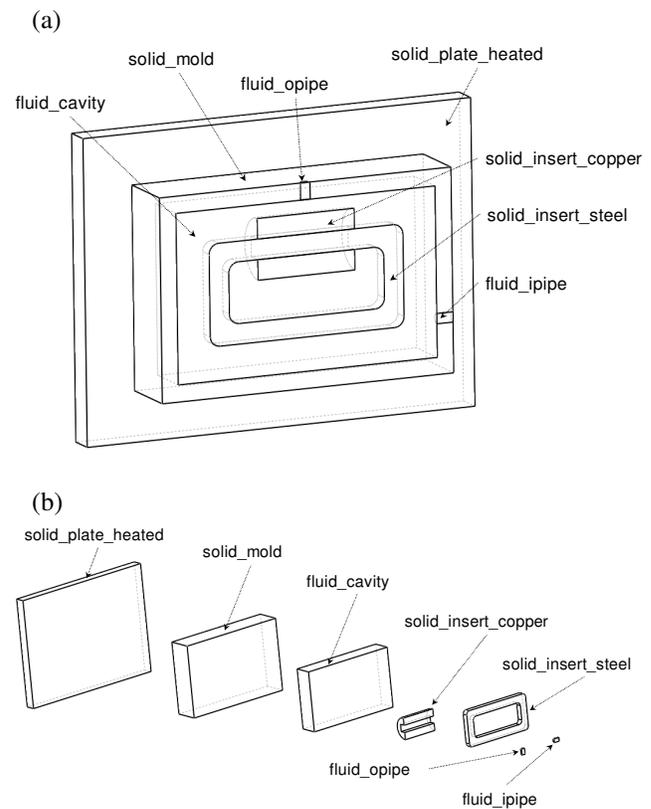
Fig. 5 Testing geometry properly labeled (a) and prepared – exploded view (b)

The CAD geometry preparation is a crucial operation that must be done by the end-user, since only at this stage it is feasible to select regions, which will be taken into consideration during the computation stage.

B. Case creation

The next step is the case creation via developed Web

platform. In order to perform that the following steps are required, Fig. 6:
- connection to the defined Website;
- login;
- browse local directories for the prepared in the previous stage the CAD geometry;
- selection of the computational module – at the moment applications belong to the Web platform allow running calculations in two different modules: high accuracy or optimize speed. Each module consists of specific tasks. Each task definition can employ different application or use it in one of many possible ways (e.g. by using specific configuration files);
- upload – it finally creates the case.
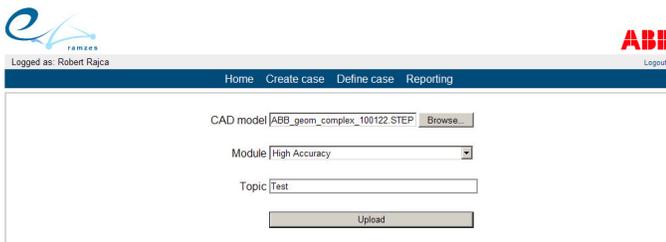
Fig. 6 Case creation page

Geometry of the product and its mold is uploaded via the Web platform as a file in a well known and widely used "step" format.

C. Analysis of the CAD geometry

When the upload is successfully finished the CAD geometry is automatically (without any further user interaction) analyzed to detect how many elements (parts) of each type (e.g. fluid or solid type) it contains. This stage is extremely important due to the saved data will be used during the meshing and solving operations. In addition based on that information the specific Web page allowing entering process parameters will be created. The actions defined and performed in that stage are invisible for the end-user.

D. Automated geometry discretization

The solution for (1)-(11) is searched by applying a control-volume-based technique to convert the governing equations to algebraic equations that can be solved numerically. This means that the solution domain (including mold walls, mold interior, cavity interior and possible inserts) is decomposed into small control volumes (or cells), and discrete values for each cell center is searched by integrating the governing equations over the faces of the cell.

Geometry discretization (mesh generation) is the second fully automated part of the entire tool. The process of mesh generation can be explained as geometry decomposition into finite number of elements – in the described tool: control volumes. It has long been considered as a bottleneck in numerical simulations due to the lack of fully automated mesh generation procedures.

During the tool development this stage was recognized as

the most challenging part of the job. Mainly it was related to complex CFD physics phenomena taking place and significantly different geometries that might be uploaded by the end-users.

Automated discretization procedure is initiated and controlled by its own Pre-processor Launcher. The mentioned automation at the discretization stage is ensured by the script – a sequence of consecutive commands, which gives orders to the meshing software (commercial software named HyperMesh). Thanks to that the Pre-processor is able to not only recognize and import the CAD geometry but also perform the following actions on the geometry:
- cleaning and repairing (removal of holes, fillets, intersections, overlapping surfaces, etc.);
- discretization of the computational domains in accordance with the rules stated in the script. Different regions can be meshed with different methods. It is possible to obtain both non-structural and structural mesh;
- set-up of boundary conditions (e.g. inlet, outlet, convection etc.) based on the specific part names;
- export for the Processor (Fluent) in the "cas" format – the output file includes discretized, correctly labeled regions with boundary conditions properly assigned.

Finally, the files generated by the Pre-processor are stored safely in the process folder and might be used when the Processor Launcher is free to accept another task.

(a)

(b)
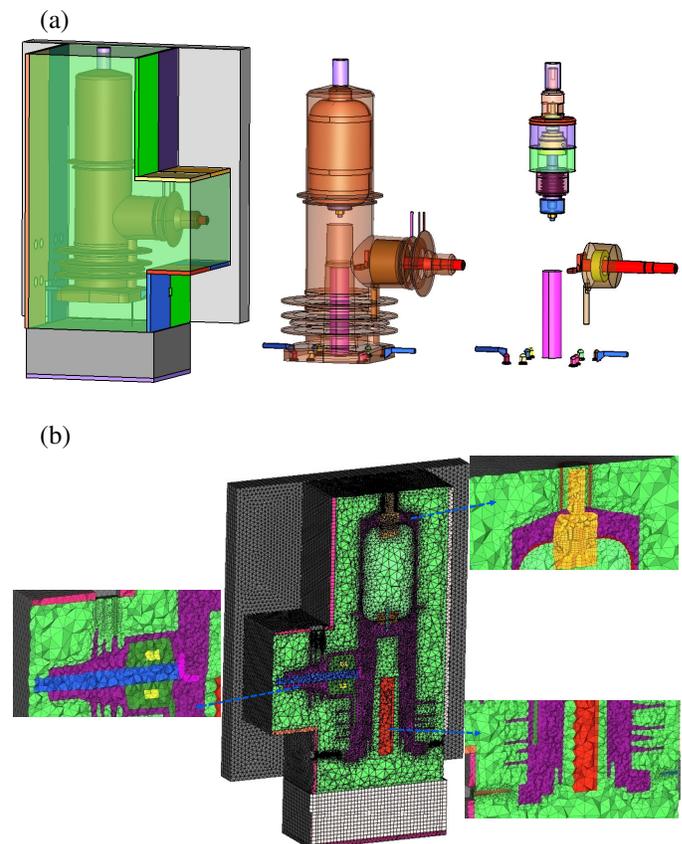
Fig. 7 Example of the geometry complexity (a); meshing result – discretized geometry (b)

It should be stressed here that the Pre-processor is able to perform all mentioned actions only when the regions and their names are well defined in the very first stage – CAD geometry preparation.

An example of the highly complex geometry that was tested (was uploaded and computed) with using developed tool is presented in Fig. 7a. The geometry consists of typical parts like cavity, mold, insulations, heater but also includes many inner parts made of different materials.

The discretized geometry consisted of above 1.5 million of elements of mixed type, Fig. 7b. The whole automated meshing process of the presented example takes approximately 45 minutes with using workstation equipped with 2 x 2.5 GHz cores and 10 MB of RAM.

This is one of the biggest advantages of the presented simulation approach – end-users can focus on solving real engineering problems and not on model discretization. In current approach only the meshing operation takes days or even weeks to experienced CFD engineers.

E. Process parameters definition

After the proper CAD geometry preparation, verification and geometry discretization end-user has to provide for the given process all the necessary parameters like the initial temperatures, velocities and material properties. Therefore the system creates dynamically (depending on geometry complexity) the Web page to allow entering all required data for all detected parts, Fig. 8.

Fig. 8 Case definition

Submitting the process parameters saves them in the process folder and then the automated simulation process can be started. Automated simulation is based on the concept of Watcher program, observing the progresses (like 'ready to start'/ 'work in progress' / 'finished') of all the simulation tasks and the availability of Launchers (like 'busy' / 'free to run'), which perform the specific tasks. The Watcher is configured on a launch-time for the specific type of the Launchers given in the parameters list. It reads the database and checks if any task is ready for the Launchers on its list. Each Launcher is designed to have three main methods – Pre, Launch and Post. Those methods are responsible for:

• preparation of the starting directory for the specific program of the Launcher;

• launching that program;
• cleanup and file management after the program is finished.

When the Launcher accomplishes job it marks the task as done and is ready to accept another task.

F. Automated computations

The next step is computation (alternatively named solving or processing). It is the subsequent, fully automated part of the developed tool.

As there are two fluids present in the mold filling stage (namely resin and air), multiphase flow modeling is required. One of the main interests in the reactive molding modeling is to know whether all and when different regions of the mold are filled, and thus the volume of fluid method (VOF) is used to predict accurately the location of the interface between the resin and air. The VOF formulation relies on the fact that two (resin and air) or more fluids are not interpenetrating [12]. In the VOF approach the volume fraction of the resin a in each cell (i.e., $a = 0$: no resin in the cell, $0 < a < 1$: a partly filled cell and $a = 1$: the cell full of resin) is solved from a conservation equation

$$\frac{\partial a}{\partial t} + \nabla \cdot (a\bar{u}) = 0 \qquad (12)$$

The volume fraction of air b is, of course, the complement of a, (i.e., $b=1-a$).

In the numerical solution of the equations, implicit first order time discretization is used, and for the convection terms first order upwind discretization is used. For the material properties (i.e. ρ, η, c_p, k) volume fraction averaged values in each cell are used. Initial values and boundary conditions must be also defined before calculations. In setting boundary conditions for the model the most important issues are the definitions of the appropriate values of the inlet, the outlet and the mold walls. In addition, appropriate material properties like thermal conductivity, specific heat, density, viscosity and curing kinetics must be measured and modeled for the used epoxy system.

The computational method described above to model the filling and curing stages of the reactive molding process has been implemented within a commercial CFD package Fluent. The mentioned CFD code does not have an option for definition of reactive nature of the simulation system such as epoxy resin; therefore it was necessary to implement in the Fluent software the models describing viscosity changes and reaction kinetics of thermosetting material as external user defined subroutines.

The computation process is initiated and controlled by its own Processor Launcher. The mentioned automation at the CFD modeling stage is ensured by the script, which gives orders to the CFD software. From the whole tool functionality point of view it is crucial that this script is generated automatically by the Processor Launcher. This operation depends on the considered product geometry (more precisely CAD geometry) and process parameters defined by the end-

user. In other words the input data provided by the user via the Web page are translated to the script language. That task is done when the Processor Launcher runs its Pre (Launch preparation) method.

At the very beginning of the computation stage the model geometry, discretized (meshed) in the previous stage, is imported into the Processor. Next, the following actions are executed:

- Model preparation, which is based on the mentioned user-defined information. This includes setting of:
  - boundary conditions (injection velocity, heating temperature etc.);
  - initial conditions (initial temperatures);
  - operating conditions;
  - materials constituting the particular geometry parts (physical properties definition).
- It is worth stressing that the model set-up described above is performed according to the rules, which strictly define the way of parts labeling at the CAD geometry preparation stage.
- Solver configuration related to the numerics, which ensure reliable and accurate CFD computations. This concerns choice of proper solver parameters and mathematical models suitable for the analyzed problem. The nature of reactive molding process is very complex and hence one has to consider many phenomena simultaneously (3D multiphase mass flow, course of the curing reaction, coupled heat transfer, exothermic effect resulting from the curing reaction). In this connection both the models built-in in the Processor as well as the ones extending the standard Processor capabilities (e.g. curing kinetics model) are used.
- Stable computations (represented mainly by solution convergence), which are controlled automatically. This solution stability was one of the biggest challenges and simultaneously achievement of the developed tool. It should be stressed that this is quite big issue even in the case of computations run manually. One should also keep in mind that all steps required at the complex processing stage are executed in the background and hence are invisible to the user.
- Results export.

All the mentioned operations are running in batch mode that allows saving total computation time, which remains one of the end-user requirement.

G. Automated post-processing and results visualization

Post-processing is the next fully automated stage of the presented approach.

This stage gives users complete insight into their fluid dynamics simulation results.

The final report we created with using macros. We recorded the interactive steps in a master session. Then file was used for replay and re-use with similar cases. It allows creating images, charts, tables, and reports automatically for different simulated cases and their results.
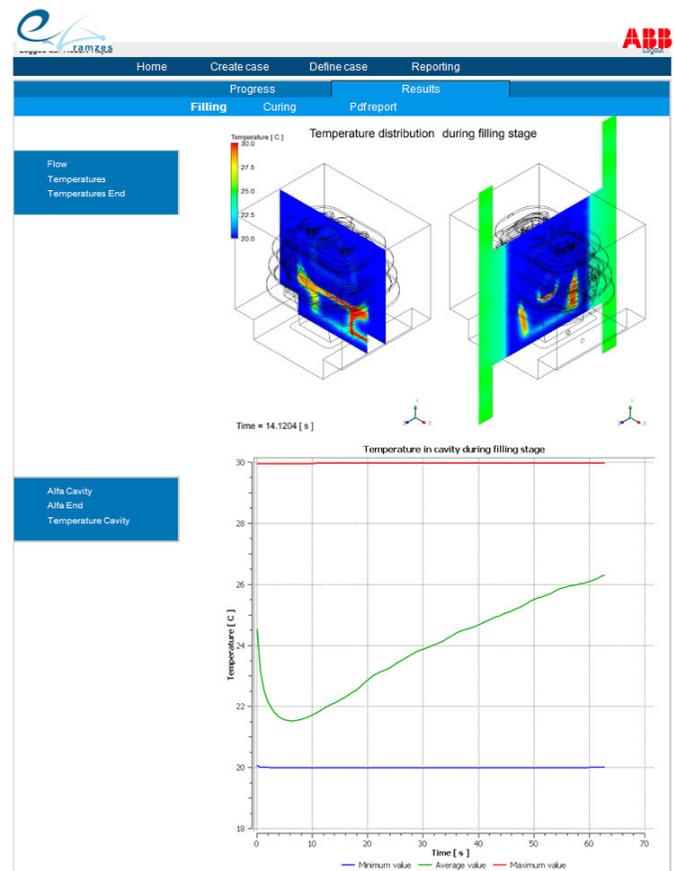
Fig. 9 Reporting page – filling stage

Data produced by the Processor are finally used to visualize results via the Web page and to create the printable "pdf" version of the final report. Results are formatted according to the user requirements and present the following useful information:

- Animations:
  - Resin flow pattern during filling stage;
  - Temperature distribution during filling stage, Fig. 9;
  - Temperature distribution at the end of filling stage;
  - Degree of curing during curing stage;
  - Temperature distribution during curing stage;
  - Temp. distribution at the end of curing stag, Fig. 10;
- Graphs:
  - Degree of curing in cavity during filling stage;
  - Degree of curing at the end of filling stage;
  - Temperature in cavity during filling stage, Fig. 9;
  - Degree of curing in cavity during curing stage, Fig. 10;
  - Temperature in cavity during curing stage;

The final report allows end-users making decision if the process and/or the product design are correct or not. The acceptance of the obtained results means the end of the tool work. In the opposite situation the end-user has two options, namely:

- to modify the process parameters - it does not require the CAD geometry to be uploaded once again;
- to redesign product or/and mold and consequently to upload the new CAD geometry.
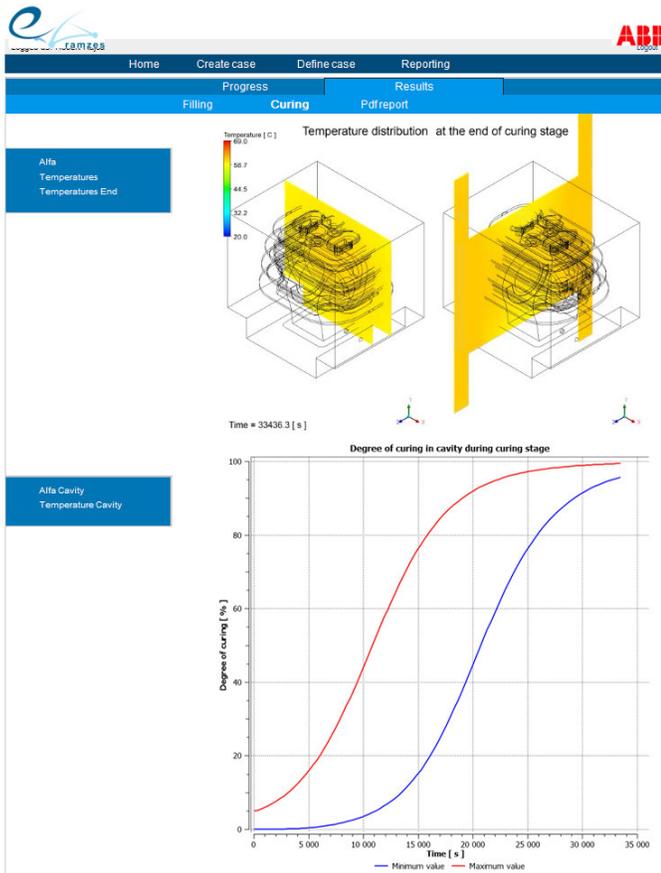
Fig. 10 Reporting page – curing stage

One of the provided benefits of the developed approach is the reporting page that can be easily modified exactly according to the end-user requirements and expectations. It is possible thanks to selecting commercial software CFD Post that allows to utilize scripting language to create the final report.

To save the computation time the CFD Post is running in batch mode as well. This functionality is extremely important due to the relatively long computation time. Generating one animation takes around one hour and requires working station equipped with high number of RAM – more than 8 GB.

IV. CONCLUSIONS

The presented novel Web-based, CFD tool can be successfully utilized for new products/processes design as well as for optimization of the existing ones. It provides sufficient information regarding epoxy resin flow and curing kinetics phenomena.

Thanks to the CFD meshing and solving stages automation it is possible to save the simulation time and eliminate, essential in the traditional approach, high user knowledge and experience in that field. The other issues are the process repeatability meaning manual-error resistance, user-friendliness and unlimited access to the tool.

Probably the biggest advantage of that tool is fully automated meshing procedure. The large number of internal components makes this stage really challenging.

All of that lead, on the one hand, to decreasing of development time of new products manufacturing in the reactive molding technology and on the second hand to improving quality of the epoxy components.

The presented approach can be easily adapted to solve other highly complex physical phenomena via Website and it that way may influence on faster development of the huge range of power products.

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