Outstanding problems of numerical simulation of the process of injection molding of PIM-feedstocks and component quality

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Abstract. Based on the experience of foreign colleagues studied in publications and own exploratory work, the authors offer their own vision of the current knowledge and problems of numerical simulation of the injection molding process of feedstocks in PIM-technology. The results of the simulation of the injection molding of challenging component are presented in the Autodesk Moldflow software package.

1. Introduction
Three branches of modern metallurgy, Powder Injection Molding (PIM, MIM), Thixoforming and Thixomolding, united into the established metallurgy of thixotropic metals, are attributed to both new special casting methods and new powder metallurgy (PM) methods. During molding, the materials used, which have previously been given thixotropic properties, are molded in a two-phase (solid-liquid) state, which is characterized by the non-Newtonian behavior of the slurry flow. The flow behavior is influenced by numerous factors of the process; in particular, the behavior of the flow depends on the loading history and time. According to the data obtained from the literature, it is easy to establish that theoretical models for such deformable solid-liquid materials are still in the development stage, and the used constitutive models are built on the basis of experiments. Combining the advantages of injection molding of plastics and the strengths of PM techniques, PIM technology makes it possible to obtain, almost without waste, exact products of complex geometric configuration from metal and ceramic powders, possessing the required set of properties and optimal cost in serial production. The versatility of the technological methods and techniques used to work with powder fillers of different nature stimulated the rapid growth in the use and development of the scientific bases of PIM technology in industrialized world, and attracts more and more attention of Russian engineers in recent years [1–4].

In PIM, only one among the main ones but, according to experts, the determining stage of the technological process is the stage of injection molding of a polymer melt filled with powder – when the slurry is spontaneously structured during the molding process. A portion of the slurry, prepared according to certain criteria of suitability for fluidity and molding under conditions of intensive heat exchange, is injected into the metal mold. For the successful implementation of such a method of forming a shaped casting from powder, a proper assessment of the properties of a solid-liquid material during deformation is necessary. The obtained semi-finished piece at this stage is called the “green” part; it is its quality that largely determines the quality of the final part. In a high-pressure casting machine, specially designed for the injection of slurry, the feedstock, a mixture of a multicomponent polymer bond and powder filler [1], strictly controlled by composition, is heated in the barrel to the
melting temperature of the binder and is brought by the screw to a condition of a viscous suspension with evenly distributed filler in it, and capable under the influence of excessive pressure of smoothly moving through all the cavities of the mold.

The metal tooling used for the manufacture of parts is an expensive mold with the shaping cavities of varying degrees of complexity, run channels, supplemented by various heating and cooling systems for the elements of the mold, a casting ejecting system, etc. Under these conditions, it is extremely important to choose the geometrical configuration of the casting cavity, consistent with the drawing of the part, and the casting conditions corresponding to the design of the mold, ensuring the production of defect-free castings. Compressibility and complex rheological behavior of the cast material with non-Newtonian properties under conditions of intensive heat exchange and solidification in channels of variable cross-section greatly complicate the design of tooling.

PIM manufacturers often have to find the right design and engineering solutions (DES) only by hit-and-miss method, as a result of which, when the mold is put into operation, they experience considerable difficulties in manufacturing defect-free castings [2–4]. The quest for the most efficient and rational DES, which allows to obtain defect-free final parts, the quality of which, as established, is 75–80% dependent on the quality of the shaped components, necessitates the use of numerical simulation of the injection molding process at the mold design stage.

2. Theoretical background

Since one of the phases of the polymer-powder mixture in the casting process is in the liquid state, and during injection, it is the slurry flow (feedstock melt) that is considered, the modeling of the injection molding process is the subject of hydrodynamic study of multiphase, spontaneously structured, and therefore thixotropic at the stage casting, media.

The main tasks of hydrodynamics as the science that deals with the motion of fluids is to determine the fields of distribution of velocities, pressure and temperature of the “fluid” in the studied space at any time. To determine these parameters, the following equations are traditionally used: the continuity equation expressing the law of conservation of mass of a fluid; the Navier-Stokes equation, expressing the law of conservation of the amount of the motion of fluid; the energy equation expressing the law of conservation of energy of a fluid; the equation of state (the constitutive model of the processed material), or as it is also called, the “closing” equation connecting the temperature, pressure, and density of the material being molded (PVT behavior).

The feedstock melt is a suspension, one of the phases of which is a dispersed filler in the form of solid powder particles, and the other is a liquid multicomponent polymeric binder. Based on this, there are 3 main approaches today to modeling the process of casting PIM-feedstocks [5]:

1) The feedstock melt is considered as a single-phase medium possessing effective macro properties of the suspension: thermal and physical properties, viscosity, equation of state, etc.

2) The particulate filler is considered as a pseudo fluid, and the flow of a two-phase medium, in which both phases are liquid, is simulated.

3) The simulation of a multiphase medium in which both the powder filler and the components of the polymeric binder are represented by fluids.

The second and third approaches, converting the suspension into an emulsion, require a larger amount of input data and the use of more complex mathematical models in comparison with the first method. Considering the flow of multiphase fluids, including suspensions, the mathematical description of the process uses the conservation equations for each phase, as well as adding new variables and equations describing the interaction of the phases with each other and characterizing the content of each component in the mixture, for example, concentrations or volume fractions of components.

The works [6–8], performed by modeling a multiphase medium, are focused on predicting the redistribution (liquation) of the feedstock components in the “green” part. The local excess of one component of the compound and, accordingly, the lack of another not only make it difficult to predict the change in the viscosity of the powder slurry during the injection molding process, but also lead to
the formation of pores or uneven shrinkage (warpage) of the part at the stages of debinding and sintering, and local decrease in physical and mechanical properties of the product.

According to some foreign experts [5], the simulation of multiphase flow is consuming computing resources and time and, therefore, in practice it is not advisable for everyday use in the design of molds. However, in the matter of compound components redistribution evaluation during the casting process, the following solution is proposed: adding additional models to the existing mathematical models of single phase flow motion, which allow predicting the distribution of the components of a polymer powder mixture based on an assessment of the results of a single-phase flow simulation. Such models include the diffusion model [5], [V. Bilovol (2003), Ph.D. thesis], which is used in the software package SIGMASOFT®; “suspension balance model” (SBM) [9], which is used in the Moldflow software [Autodesk knowledge network. Suspension balance model from www.help.autodesk.com].

A team of authors [10] presented one of the basic works on simulation of the process of injection molding powder slurries. In this work, the feedstock melt is considered as a single-phase medium, endowed with effective suspension properties. The main emphasis is on the description of the rheological behavior of the feedstock. In the mathematical models used, the authors consider the presence of a yield strength and the presence of a so-called “slip” layer (“slip phenomena”), a characteristic phenomenon during the flow of highly filled materials, in which a thin layer of pure bond appears, which is formed under the action of shifts at the contact interface of the melt and walls of the mold. The 2.5D modeling approach for thin-walled PIM products used by the authors of [10] simplifies the solution of the proposed mathematical model with Hele-Shaw approximation, but at the same time limits the use of the developed PIMSolver® software for products that are not thin-walled and have bulky elements.

For the above works and a number of other publications in the field of simulation of the injection molding of polymer-powder compositions, attention is paid to the rheological behavior of the suspension. Most foreign colleagues [10–12] tend to use the Cross-WLF model, supplemented by the Herschel-Bulkley (HB) model and its various modifications. The use of the Cross-WLF+HB allows describing reversible transitions in the behavior of the thixotropic material in low shear rates most adequately, which leads to an increase in the accuracy of calculations. In the description of the rheological behavior of the dispersed systems under consideration, it is necessary to take into account the effect on viscosity not only of thermodynamic criterion and shear rate, but also of the time. In concentrated suspensions under the action of stationary shear, the effect of thixotropy appears, which is associated with structural changes in the dispersed system, leading to a change in viscosity during relaxation with a change in shear pull rate [1–3].

Components of the polymer bond experience a significant thermal expansion upon heating and shrinkage during cooling. For the description of PVT data of the feedstock, 2-domain Tait PVT-model is most often used [4, 10, 11, V. Bilovol (2003, Ph.D. thesis), K. Kate (2012, master thesis), V. Raymond (2012, master thesis)]. The change in the specific volume of the feedstock must be considered when selecting the parameters for the filling and the packing stages of the injection molding and when designing the mold.

An important issue for numerical simulation is to provide the mathematical models used with correct data on the properties of the polymer-powder compound. There is a significant difference between the values of the parameters in the process and in the research of the mixture with modern techniques. For example, the heating and cooling rates when studying with the DSC method and when determining PVT data, as well as changing the derivative of the shear rate when studying viscosity on the rheometers, can differ significantly from the real ones. The correctness of the obtained data on the properties of the feedstock [13–17] and, as a result, the correctness of the results of numerical simulation significantly depend on these parameters. At the moment, a clear boundary between the sufficient accuracy of the measured data on the properties of the polymer-powder compound and the acceptable accuracy of the computational experiment has not yet been established.
For the computational experiment, the value of the heat transfer coefficient between the melt and the mold, which will depend largely on the composition and properties of the compound and the surface quality of the mold cavities, is extremely important. The publications [18] and [V. Raymond, 2012, master thesis] thus give significantly different values of the heat transfer coefficient, which confirms the existence of this problem and the need to solve it.

3. Experimental procedure
In one of the challenging products, it was possible to successfully apply the obtained knowledge in the field of numerical simulation of the technological process under consideration [1]. The study object is presented in Figure 1. No problems with the liquation of the components of the compound were found in the study object; the method of simulation of a single-phase medium endowed with effective macro parameters of a polymer-powder compound was chosen as the approach used. The preparation and conduct of the computational experiment are described in more detail in publication [1].

Using the method of differential scanning calorimetry (DSC) and the laser flash method (LFA), the effective thermal and physical parameters of the feedstock used for the manufacture of this part were investigated [19]. Based on the type of polymer binder used, on the morphological characteristics and particle size distribution of the powder filler, empirical coefficients of the most representative for this type of feedstock viscosity model (Cross-WLF) and coefficients of the 2-domain Tait model were selected from publications. Based on the feedstock processing parameters provided by the manufacturer, the injection molding process was simulated using the Moldflow software package. As Figure 2 shows, the suggested technique allowed obtaining results that rather well correlate with the observed defects in the real product. The selected area of maximum volumetric shrinkage coincides with the zone of defects in the cylindrical part of the component. The value of the maximum volumetric shrinkage of ~ 11% indicates a low efficiency of the compressing, which requires an adjustment of the parameters of the filling process at the packing stage. Since the compound has a massive part and is non-moldable for MIM, it may be necessary to change the geometry of the runner channels and the gate to prevent the run blocking before the end of the packing stage (or to use a hot runners mold).

Figure 1. On the left: a general view of the casting and sintered part, respectively. On the right: images of defects of the “green” part, obtained on the computer tomography unit [1]
Figure 2. Comparison of the results of the calculation of volumetric shrinkage with the results of metallographic study of the part. The contour marks the zone of maximum volumetric shrinkage for the calculation results (on the left) and the defect location zones in the sintered part (on the right) [1]

4. Conclusion
Currently, the issue of numerical simulation of the injection molding of polymer-powder compounds in PIM technology is adequately treated, a lot of research has been done and software packages have developed for simulation of the technological process (SIGMASOFT®, PIM Solver®, modules in Autodesk Moldflow®, Moldex 3D®, etc.). The provision of the used mathematical models with correct data on the properties of the polymer-powder compound remains an important problem.

As shown above, even in the first approximation, using relatively simple mathematical models (approaches) with an incomplete amount of experimentally measured data on the properties of the feedstock, it is possible to simulate the process of injection molding of polymer-powder slurries for the purposes of analysis and evaluation of the DES taken at the stage of the mold design.

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