# DESIGN AND DEVELOPMENT OF SIMULATION SOFTWARE FOR INVESTMENT CASTING PROCESS

ŻABA Krzysztof[1], HOJNY Marcin[1], MIZERA Jarosław[2], SITEK Ryszard[2], PUCHLERSKA Sandra[1]

[1]*AGH University of Science and Technology, Poland, EU*
[2]*Warsaw University of Technology, Poland, EU*

**Abstract**

In the paper some aspects of the practical implementation of the simulation systems computer-aided design in investment casting are discussed. Presented hypothesis and methodology are based on original solutions allowing to develop unique tools in the context of designing new technologies. This is closely related to the practical design and implementation of numerical solutions, testing and validation and in the final stage with testing in industrial conditions. An example of such a dedicated system is the DEFFEM package, whose computational capabilities are presented in this paper simultaneously with the directions of further development and implementation work.

**Keywords:** Smoothed particle hydrodynamics (SPH), finite element (FE), solidification, liquid flow

## 1. INTRODUCTION

The continuous development of new technologies, competition in the market, or pursuing a continuous improvement in the product quality makes us look for solutions to aid decision processes at the stage of production preparation. Now, it is difficult to imagine the operation of a modern industrial plant, which does not benefit from the application of modern computer aided design systems and decision aiding systems at the engineering or production stages. The computer aid to engineering work includes simulation, validation and optimisation of products, processes and production tools, virtually in all engineering domains. This has inspired the authors to take up intensive and time-consuming work related to the development of research methods and mathematical models, along with their numerical implementation. This resulted in developing a concept of modelling, which integrated the areas of physical and computer simulations, whilst providing full or partial exchange of information between those areas [1]. The proposed concept utilizes capabilities of modern thermo-mechanical simulators of the Gleeble 3800 series in the physical modelling of industrial processes, and the original simulation package DEFFEM [1], which has been under development for a few years. The whole modelling approach is rounded up by the utilization of modern testing and measurement instruments (e.g. blue light scanning systems) to verify the implemented solutions, or to get additional information impossible to be obtained with traditional methods (e.g. computer tomography). In publication [1] the mentioned methodology of integrated modelling is presented in details. In the presented study, results of model tests (physical and computer) are shown, aiming at developing a simulation tool to aid designing casting processes for critical parts of jet engines. The technology of precise investment casting in multi-layer ceramic moulds enables geometrically complicated shapes of aircraft parts, such as: turbine blades, vane segments, turbine nozzle rings, casings and others, to be recreated. These components operate under a very high pressure and often at a temperature above 1000 °C and are called critical parts of jet engines. They are made of nickel superalloys. The production process of aircraft engine parts is complex, and many material, technological, and organisational factors influence the ultimate quality. Multi-layer ceramic investment moulds are made in a multi-operational process of applying subsequent ceramic coats onto wax pattern assemblies, dewaxing, washing, drying and burning out the mould. Coats are applied either manually or by robots. After the burnout, moulds are warmed, preheated to an adequately high temperature and filled with liquid metal in vacuum conditions. The cost of the part material - usually very expensive nickel and cobalt superalloys, and the subsequent post-casting treatment operations account for a substantial part of costs (even up to 70%) of

manufacturing critical aircraft engine parts. Each of the mentioned individual processes may introduce defects (**Figure 1**), which can be either repairable or not. Therefore, the accurate quality inspection of semi products is very important.

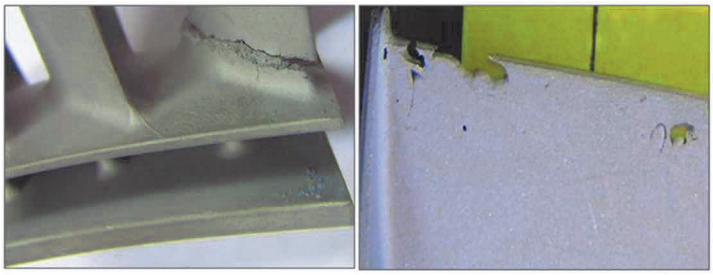

**Figure 1** Examples of casting defects (author's materials)

Wax patterns, wax pattern assemblies and multi-layer ceramic investment moulds not fulfilling the requirements - which can lead to manufacturing faulty castings - should be eliminated already at an early stage. At the moment there are no effective methods of interoperational quality inspection of a mould during execution of individual processes and a mould as a final product. Currently, moulds in a not fully identified condition are transferred to subsequent mould manufacturing operations and to the operation of filling with liquid metal. It results in losses related to yield, product repair costs, and losses arising from unnecessary manufacturing costs of a faulty mould. The situation is even more difficult, as no causal, precise, qualitative description of individual processes has been constructedso far, to enable the casting result to be predicted on the basis of the set of manufacturing parameters of the pattern assembly and the mould.The mould is still assessed post factum, after casting, on the basis of the finished product (casting) quality. Although both academic and industry-related literature is abundant in papers concerning methods of nickel superalloy precise casting, so far no methods and procedures for aiding design and quality inspection of multi-layer ceramic investment moulds have been defined, which would allow a faulty mould to be eliminated from the manufacturing line before the filling operation. The dedicated original simulation software DEFFEM |solver_3D_HYBRID included in the solver line of the DEFFEM package [1] is a component of the methodology developed. The hybrid solution is focused on the possibility of, among others, the identification of defects occurring during the solidification process in a ceramic mould.

## 2. MAIN ASSUMPTIONS OF HYBRID SPATIAL MODEL

The developed and implemented hybrid model combines the advantages of the finite element method (FEM) and the smoothed particle hydrodynamics (SPH). The governing equations of fluids in the SPH method are based on the Navier-Stokes equations in the Lagrangian form [2,3]. The dynamic particle was selected as a definition of boundary conditions [4]. These kind of particles have the same properties as the fluid particles except that the equation of momentum is not solved for them. The heat exchange between the particles occurs by conduction. The model of heat conduction is based on the enthalpy method which is given by:

$$\frac{dH}{d\tau} = \frac{1}{\rho}\nabla(\lambda\nabla T) \tag{1}$$

where: $H$ is enthalpy, $\lambda$ is thermal conductivity, $T$ is temperature and $\tau$ is time. The SPH formulation of this equation is approximated by [5]:

$$\frac{dH_i}{d\tau} = \sum_j \frac{m_j}{\rho_i\rho_j}\frac{4\lambda_i\lambda_j}{(\lambda_i+\lambda_j)}\left(T_i - T_j\right)\frac{(r_i-r_j)\cdot\nabla_i W_{ij}}{(r_i-r_j)^2+\eta^2} \tag{2}$$

where: $\eta$ is a small parameter to prevent singularity when $(r_i - r_j)$ goes to zero, $m_j$, $\rho_j$, $\lambda_j$, $T_j$ are the mass, the thermal conductivity, the density and the temperature of particle $j$, respectively, $W$ is the smoothing kernel,

index $j$ corresponds to any neighbouring particle of particle $i$. The phase transition (from liquid to solid) occurs when the particle temperature is below the solidus temperature $T_s$. In the proposed solution, the solid particles are modelled as a viscous pseudo fluid. It means that solid particles be have like fluid particles but they move under a very high viscosity. This approach is used to keep the forces impacting the solid particles and fluid particles. The solution in the form of temperature field for the FEM model was predicted by solving the Fourier equation, which in its general form can be written as follows [1]:

$$\nabla^T(\lambda\nabla T) + \left(Q - c_p\rho\frac{\partial T}{\partial \tau}\right) = 0 \quad (3)$$

where: $T$ - absolute temperature, $\lambda$ - thermal conductivity coefficient, $Q$ - heat generation rate for volume unit, $c_p$ - specific heat, $\rho$ - density, $\tau$ - time.

The model coupling the both domains (FE+SPH) is based upon a solution of coupling by fixing particles to the FE nodes (**Figure 2**). The computing procedure is performed in two stages. At the first stage calculations in the particle solution domain are performed. The FEM mesh nodes constitute the boundary condition for the particle model, and during computing they are treated as fixed particles. At the second stage, computing in the finite element method domain is performed. The temperature of particles within the exchange interface at the same time is the first type boundary condition for computing in the finite element method domain [1]. The heat is exchanged with the environment (the simulator inside) on the basis of the convective heat transfer modelled with the use of effective heat transfer coefficient [1].

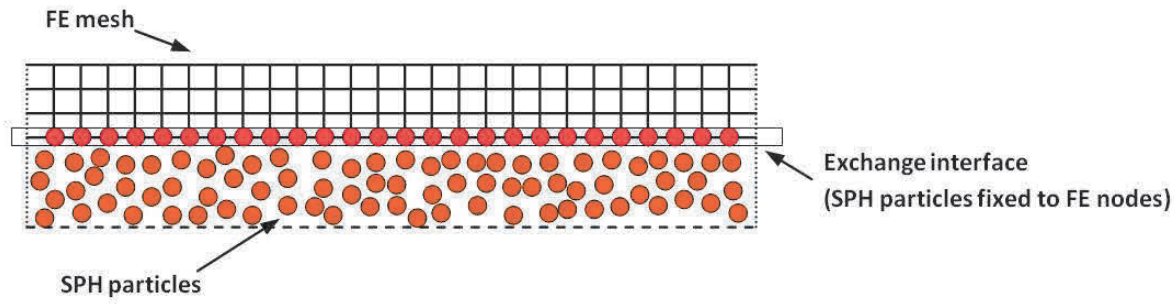


**Figure 2** Scheme of coupling both solution domains (FE+SPH)

## 3. PRELIMINARY VERIFICATION OF THE HYBRID MODEL

As part of test simulations computing was carried out for the test variant, focusing on the assessment of the implemented thermal solutions. Cylindrical specimens with diameters of 10 mm and lengths of 125 mm were tested with the Gleeble 3800 thermo-mechanical simulator [1]. The material used in simulations is medium carbon steel (C45 grade steel) and the temperature dependent thermal properties, required for the simulation were calculated by using the commercial JMatPro software based on the chemical composition of the investigated steel [1]. The liquidus $T_l$ and solidus $T_s$ temperatures of the investigated C45 grade steel are 1494.79 °C and 1412.42 °C, respectively. The simulation was oriented at the test hybrid solver and the possibility to predict defects within the volume of the sample, as well as the robustness of the hybrid solver. The specimen was heated with the resistance heating method, with an automatically controlled alternating current being introduced into the specimen through cooper grips in the Gleeble equipment. At the first stage of the physical simulation, the specimen was rapidly heated up to 1350 °C at a heating rate of 20 °C / s. At the second stage, the specimen was slowly heated up to 1430 °C at a heating rate of 1 °C / s and held at this temperature for 30 seconds. Finally, the specimen was cooled down to the nominal temperature,and after holding for 10-60 seconds, cooled down to the ambient temperature. To prevent oxidation, the specimen was put into a vacuum chamber. A transparent quartz sleeve was used to protect against a potential leakage of metal during melting. In order to find out the temperature distribution along the heating zone within the

specimen, temperatures were continuously measured at several locations of the sample [1]. A special thermocouple was mounted in the core of the specimen to give access to the radial temperature gradient. The hybrid methodology of numerical modelling consists of three main steps: At the first stage (resistance heating and melting process), the spatial **DEFFEM** |**solver_3D_TH** based on FEM is applied in order to estimate temperature distribution within the volume of the sample [1]. The temperature schedule of the numerical simulation of the process of heating, remelting and cooling the specimen was analogous as in the conducted physical simulations. **Figure 3** presents the temperature distribution field after cooling to the nominal temperature 1380 °C. On the other hand, **Figure 4A** presents the temperature distribution on the cross-section and the longitudinal section (the centre of the heating zone), and the visualisation of the mushy zone (**Figure 4B**), where the visualisation of temperature distribution was restricted to the range between the solidus temperature $T_S$ of 1412.42 °C and the calculated maximum temperature in the sample core of 1421.97 °C. This method of visualization allowed us to estimate the size of the mushy zone, which on its cross-section may be defined by the radius of ~ 2.5 mm, reaching on the longitudinal section the length of ~ 6.9 mm.

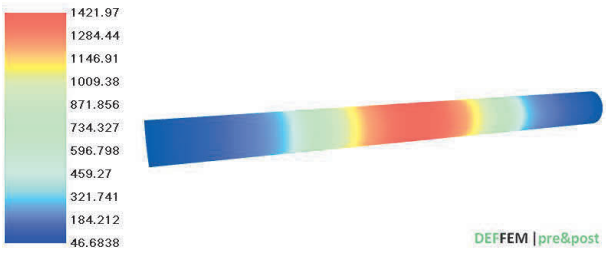


**Figure 3** The temperature distribution after cooling to the nominal temperature 1380 ℃ (spatial solution)

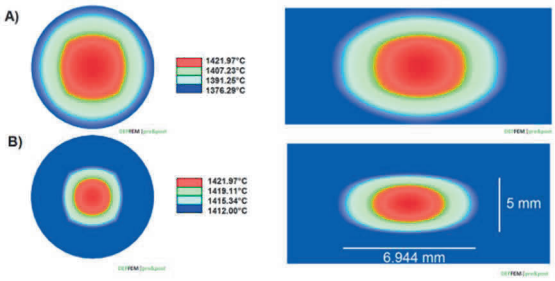


**Figure 4** The temperature distribution
A) on the cross-section and the longitudinal section of the sample,
B) mushy zone (liquid and solid phases)

When analysing the obtained results one may observe a considerable gradient on the sample cross-section (**Figure 4A**). With reference to the surface temperature of 1376.29 °C achieved during the numerical simulation, and the maximum temperature reached within the sample core of 1421.97 °C, this difference was 45.68 °C. In the conducted physical simulations, the mentioned average difference between the measured values was 40 °C [1]. Given the fact that the effect of heat exchange disturbance caused by the quartz shield was not included in the numerical model, and a constant value of the effective heat transfer coefficient was applied, the obtained results show a high compliance. In the second stage of the model procedure, new solution domains are generated. The first solution domain is the finite element mesh in the sub-surface areas of the sample. In the second solution domain, particles are generated within the volume of the sample together with their temperature initialization based on the interpolation temperature from FEM mesh nodal results. In the third stage, the developed hybrid solver DEFFEM |solver_3D_HYBRID was used to simulate the solidification process. Examples of particle temperature distribution during the solidification process are presented in **Figure 5** and **Figure 6**. **Figure 5** presents the temperature distribution on the longitudinal-section of the sample just after starting the free cooling. With reference to the determined velocity field (**Figure 7**), the solidifying metal slowly flows within the sample volume and a discontinuity in the sample centre begins to form (**Figure 5**). Intensification of the formation of the defect zone starts to be observed in the medium stage of solidification process (**Figure 6**). It is caused by a variable liquid metal flow rate within the sample volume (**Figure 8**). Three main zones can be distinguished there: the bottom, the central, and the top one with a significantly diversified flow rate. Due to the effect of gravity and the simultaneous solidification the top zone reaches the maximum values of flow rates, at practically zero values of velocity fields for the bottom zone (the solidified zone).

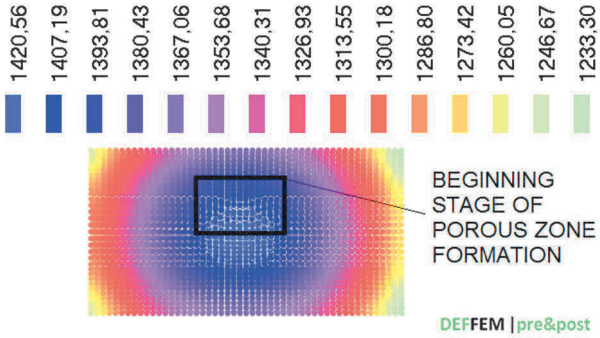


**Figure 5** Particle temperature distribution on the longitudinal-section of the sample during the solidification process (initial stage of the solidification process, particle solution domain only)

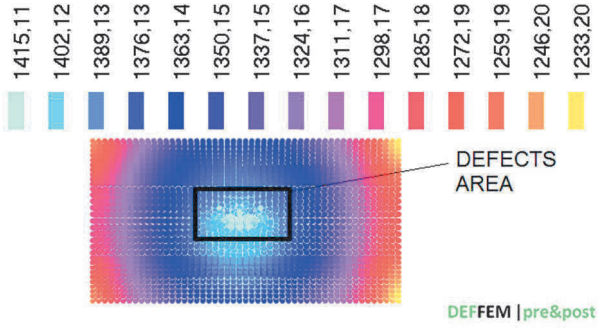


**Figure 6** Particle temperature distribution on the longitudinal-section of the sample during the solidification process (medium stage of the solidification process, particle solution domain only)

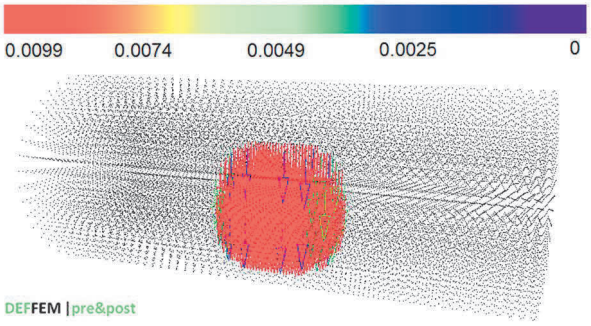


**Figure 7** Velocity field distribution within the volume of the sample (initial stage of the solidification process, particle solution domain only)

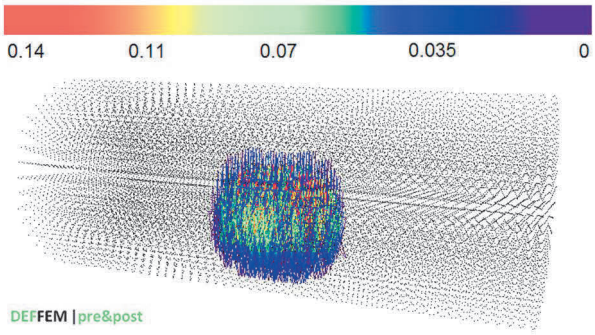


**Figure 8** Velocity field distribution within the volume of the sample (medium time of the solidification process, particle solution domain only)

The final temperature field after the completed solidification process is presented in **Figure 9.** The maximum temperature within the sample volume reached a value lower than the solidus temperature $T_S$, and the formation of a porous zone (defect area) could be observed in the sample core. The tendency to form the porous zone coincides with results of macrostructural tests [1]. The computer simulation results are promising, however the DEFFEM |solver_3D_HYBRID requires further validation tests based on physical simulations. The maximum core sample temperature of 1421.97 °C is about 9 °C higher than the solidus temperature $T_S$ of 1412.42 °C (**Figure 3**). On the basis of the maximum temperature and the solidus temperature, the size (volume) of the mushy zone was estimated. The volume of the mushy zone during the simulation of the solidification process decreases, reaching the minimum value after 0.3 seconds from the beginning of the solidification process (**Figure 10**). With reference to the results of the physical simulation, this state was achieved in the half of the time of the actual solidification process that was recorded during the experiment. According to the physical results, the solidification process took 0.6 seconds. At the beginning of the solidification process, during about 0.2 seconds, the temperature changes between the computer and physical simulations were very convergent. The process of solidification in the computer simulation finished 0.35 second faster than during the physical simulation. The main reason for such a difference is the adoption of a linear approximation of enthalpy changes versus temperature in the numerical model as well as the assumption of a constant heat effective exchange coefficient in the FEM model [1].

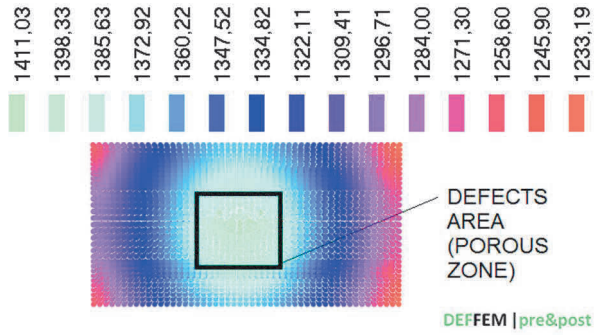


**Figure 9** Particle temperature distribution on the longitudinal-section of the sample after completing the solidification process with visible defects within the sample volume

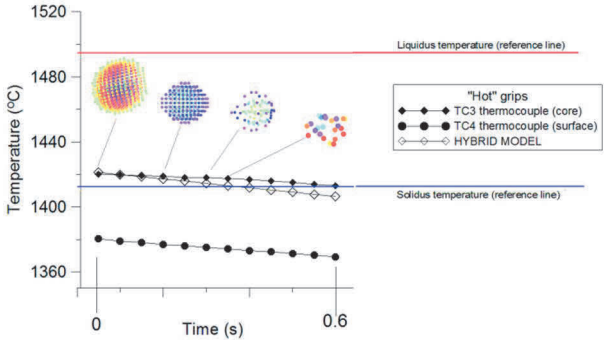


**Figure 10** Calculated and measured change in the sample core and surface temperatures (the solidification stage)

## 4. CONCLUSION

The article presents the main assumptions of the hybrid model, aiming at developing a simulation tool for precise casting and solidifying critical parts of aircraft engines in multi-layer ceramic moulds. The solidification process was calculated by applying the enthalpy method in SPH formulation to solve the heat transfer problem. The phase transition model from liquid to solid was treated by considering the effect of latent heat and nonisothermal phase change to the model of heat transfer. The conducted physical simulations of the solidification process with the Gleeble 3800 thermo-mechanical simulator allowed the developed tool to be tentatively verified for anticipating defect areas. Further work related to the developed solution will focus on making the liquid-solid phase interaction model more specific by adding a particular force between the mushy and the solid phases, or the procedure of particle grouping and taking into account its movement within the mushy zone (liquid and solid phases).

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