SPECIAL CONSIDERATIONS RELATED TO THE DIGITAL TWIN DEVELOPMENT FOR AN EVACUABLE SMALL-SIZED DIRECT JOULE HEATING MELTER DESIGNED BY PA MAYAK

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The article discusses the key features associated with the development of a digital twin (DT) for a small-sized direct Joule heated elter designed by Mayak PA and also describes a set of mathematical models constituting to the digital twin of the product and reflecting the relationship between the models and their development flowchart. The article presents the key performance characteristics of the considered melter, the data on which were required to develop the DT. Vitrification units are complex high-tech industrial products involving multiple interconnected physical processes. The article touches upon the advantages of digital platforms and their application in the context of automated collection and exchange of data between the computer models. The paper considers the application of the CML-Bench® developed at SPbPU as such a digital platform.

Keywords: *digital twin, digital platform, validation, small-sized removable melter, drain device, Joule heating, induction heating, borosilicate glass, vitrification, high-level waste, radioactive waste.*

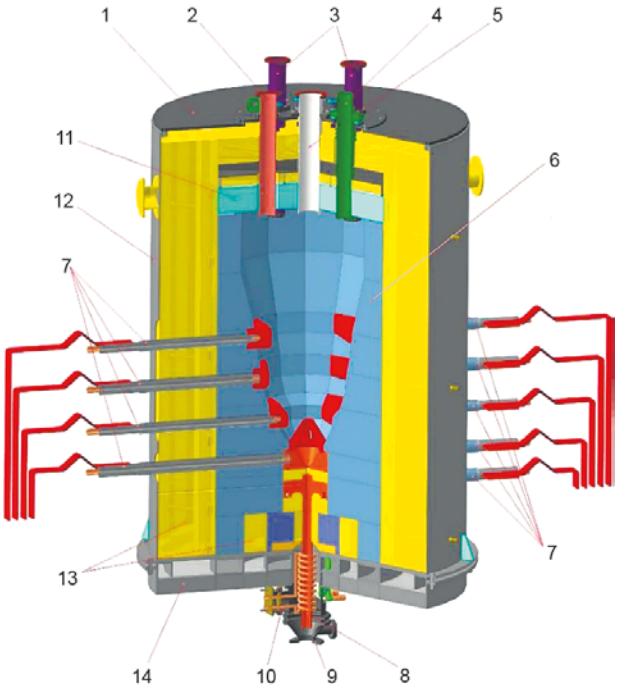
Introduction

Nuclear power plant operation results in spent nuclear fuel (SNF) and radioactive waste (RW) generation. Their conversion into a form suitable for transportation, storage and disposal is viewed as an important task for modern science and technology.

Liquid high-level waste (HLW) is reprocessed using vitrification technology, i.e. they are immobilized in a stable glass waste form. Since 1987, industrial vitrification of HLW generated from SNF reprocessing has been carried out at Mayak PA in purpose-designed high-performance furnaces with direct electric heating [1]. To further improve this method, a new vitrification unit is being developed - a small-sized removable melter, which is a vertical glass melting furnace of a conical-cylindrical shape with electric (Joule) heating and an induction-heated bottom drain device [2], [3]. The developed design has a number of important advantages compared to the currently operated equipment.

A prototype of the removable small-sized melter is schematically shown in Figure 1.

Due to the complexity of physical-mechanical and physical-chemical processes, the development of vitrification units are associated with high resource costs for redesign based on the results of full-scale tests. Therefore, to reasonably reduce these costs, software suites and tools for digital (virtual) experimental studies are being developed,



1 — lid, 2 — thermocouple branch pipe, 3 — glass frit feed units, 4 — gas duct, 5 — solution feed unit, 6 — ceramic refractory melting bath, 7 — current leads with electrodes, 8 — drain outlet channel, 9 — inductor body, 10 — inductor, 11 — arch, 12 — body, 13 — thermal insulation, 14 — base

Fig. 1. Schematic design showing a prototype of a removable small-sized melter designed by Mayak PA:

in particular, for those enabling related and multiphysical calculations providing high accuracy in terms of the key characteristics.

The Rosatom State Corporation is actively introducing digital technologies in projects dealing with decommissioning of nuclear facilities and RW management seeking to improve safety while optimizing the timing and cost of the work in progress. In particular, they are viewed as a way to preserve data and provide information to support decision making on the development of the Unified State System for Radioactive Waste Management [4].

In literature, complex products consisting of a large number of interconnected systems and units influencing each other are often referred to as Systems of Systems (SoS). In the design development and operation of complex technical systems, methods of model-based systems engineering and the digital twin technology are quite actively used [5]-[10]. This concept is based on the idea that instead of separate independent models of subsystems and components, the design development process can rely on a single digital model combining all their characteristics and properties. The national standard Digital Twins of Products [11] developed by SPbPU and RFNC VNIIEF specialists under the supervision of A. I. Borovkov defines some general provisions supporting DT development for both newly developed products and those developed earlier or those already being in operation. The standard requires the development of a system (family) of multidisciplinary mathematical and computer models (CM) describing the behavior of a complex device under various operating conditions. Obviously, information exchange should be provided between its elements as well, for example, using the digital CML-Bench® platform for DT development and application that was designed to solve such problems [12]—16].

Digital platform CML-Bench®

Development of a single digital model describing the behavior of an actual industrial facility requires an adequate software and hardware system, in which computing hardware is integrated with the results of computer design development, modeling and engineering, systems for data generation, collection, processing and transmission, as well as some visualization tools.

To develop and apply such DT, SPbPU uses a proprietary product CML-Bench® — the Digital Platform (DP) for Digital Twin Development and Application, which is a client-server web application involving a user interface, a server part, a database management system and a solver service.

The main functions of the DP can be summarized as follows:

- storage and management of calculation data (mathematical and computer models, results of their verification and validation, solutions to multidisciplinary problems, mathematical, computer and supercomputer modeling results, multivariate digital tests, including research performed on purpose-developed virtual stands and test sites, solutions to optimization problems);
- development of a requirement traceability matrix and its adjustment, development of target indicators and resource constraints, in particular, the technological and production ones;
- automated initiation of digital testing processes and monitoring of their progress, as well as processing of their results (postprocessing);
- management of computing capacities both as it comes to the computer network and the supercomputer capacities;
- management of engineering software licenses (advanced domestic and foreign CAE (Computer-Aided Engineering) systems).

Fig. 2 shows the DP structure in terms of its application for digital (virtual) product testing.

The main tools that aid in organizing the testing using the platform are as follows:

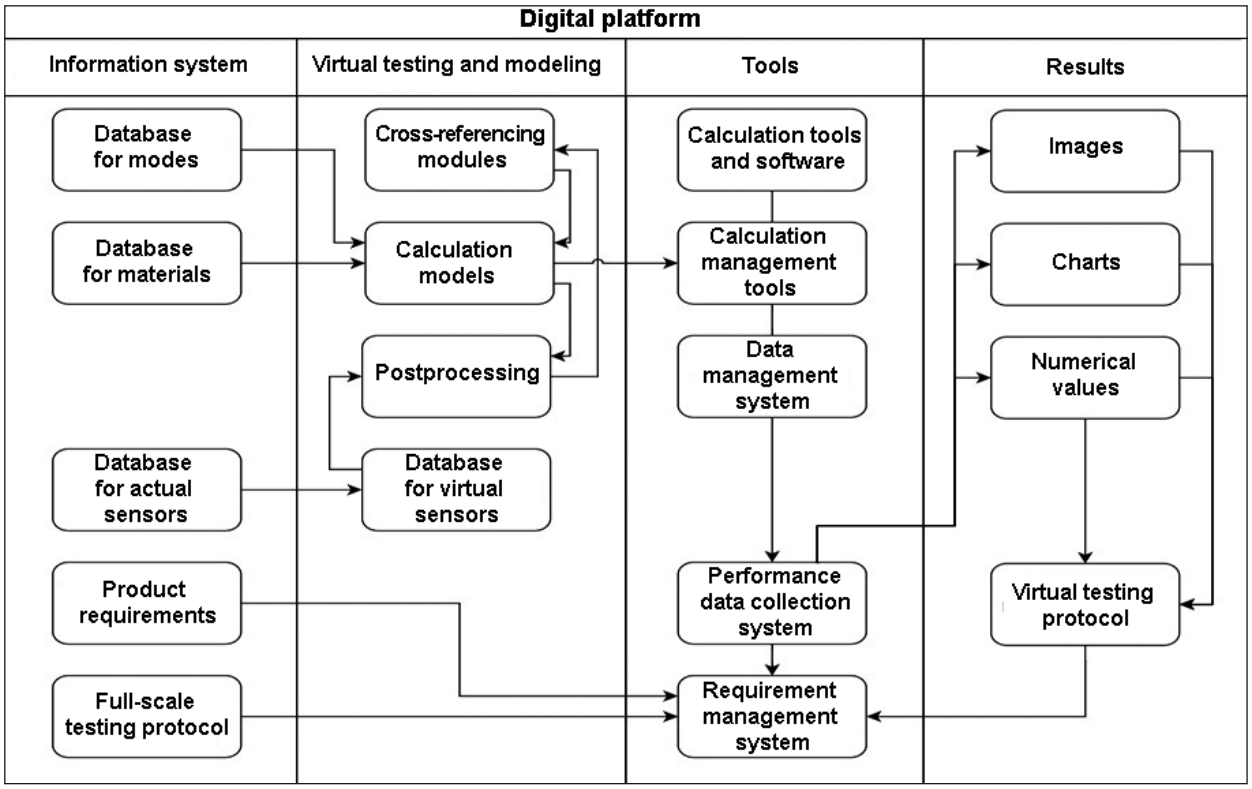


Fig. 2. Structure of the digital platform

- tools providing the generation of calculation models, preparation of input data and establishment of initial conditions;
- computational software applied to solve the problems when multidisciplinary (multiphysical) processes have to be modeled;
- tools enabling collection, processing and visualization of data obtained from the modeling results;
- tools enabling automated transfer of information among the components of one or more CM.

An informed choice of engineering software (SW) for computer modeling is based on the evaluation of requirements to each CM, assessment of capabilities of software components involved in computer modeling as well as possibility of integration among various SW and their program modules for ensuring proper data transfer among related models. Clear understanding of the CM system architecture is viewed as an essential component of this process, which takes into account specific nature and peculiarities of industrial equipment and its operation.

To select a proper software tool, the following characteristics should be taken into account: settings should be flexible enough given the complexity of the simulated physical-mechanical and physical-chemical processes; calculations should be run in parallel; graphical user interface should not be needed to run software modules; automation tools should be available primarily supporting the generation of automated calculation chains, which often requires the development of specialized interfaces. One of the main requirements established for computational software is its ability to solve multidisciplinary (multiphysics) problems. The only constraint that determines whether CAE systems can or cannot be integrated in the framework of the CML-Bench® digital platform is the feasibility of running the CM software in a command line mode.

The digital platform helps create a unified and transparent system for storage and management of data, models and computer modeling results ensure integration among computer models in terms of data storage and information exchange and validate data using results of experimental studies and full-scale tests.

Digital model architecture

To determine the characteristics and properties of a system, there is a need to carry out its detailed decomposition into subsystems, identify the main ongoing physical and mechanical processes, as well as its target (individual) indicators. In this way, requirements are set for potential functional DT blocks, which are represented by mathematical and computer models. Further, in accordance with the type of tasks at hand (modeling of hydrodynamics, heat and mass transfer, electrodynamics,

mechanics of deformable solids and strength), their complexity and the dimensionality of the problem, the discretization step in space and time, a set of mathematical and computer models should be built.

In cooperation with Mayak specialists, main units have been identified which functional characteristics should be described using mathematical and computer models:

- dosing device;
- housing;
- crucible (melt zone);
- main electrodes;
- cooling system;
- drain unit;
- induction heating unit;
- sensors.

The same models should also specify the purpose and the behavior of the product in the following main furnace operating modes:

- start-up using starting heaters;
- dosing and heating;
- glass melt holding;
- emergencies (glass melt holding without current supply);
- drain modes: initiation and shutdown.

In the course of decomposition, a list is compiled containing the monitored key characteristics of the selected units and parameters of the technical system used for CM validation, including a comparison of the results of digital (virtual) testing and the target parameters determined in accordance with the requirements specified for the unit under consideration.

Fig. 3 presents the system decomposition in the form of a relationship tree with the key parameters of the technical system used for model validation highlighted in green.

When mathematical and computer models of high-temperature industrial facilities are developed, special attention is paid to temperature-dependent material properties, such as electrical conductivity, density, viscosity, thermal conductivity and heat capacity, since they affect the processes occurring in the crucible. For example, heating increases glass electrical conductivity [17], temperature affects glass density and facilitates natural convection (i. e. causing mixing of the glass). The non-linear relationship between melt viscosity and temperature [18] has a significant effect both on convection in a glass-filled crucible and on arrangement of controlled discharge of the melt via an induction-heated drain [19]. In cases when the thermophysical properties of materials are not known or were defined in a limited temperature range, the available experimental data should be processed based on various approximation methods [20].

In addition to investigation and identification of physical and mechanical material properties, mathematical and computer modeling should include an analysis and consideration of all physical processes evolving in the furnace. For example, in addition to glass heating with electric current (Joule heating), it is also necessary to take into account the hydrodynamic processes evolving in the melt. Under the glass melting process, one should also take into account the thermal radiation from the melt surface, as well as the processes taking place in the vapor-gas phase. When induction processes are modeled, one should also take into account the influence of the skin effect [21], which manifests

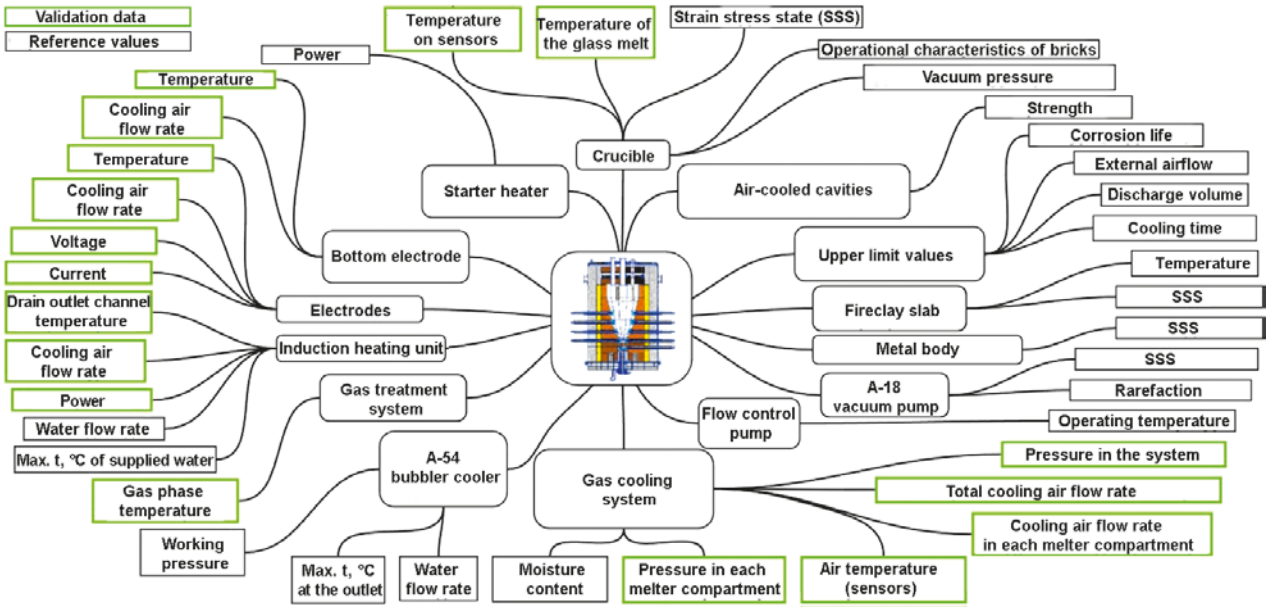


Fig. 3. Characteristics and parameters of a technical system for computer model validation

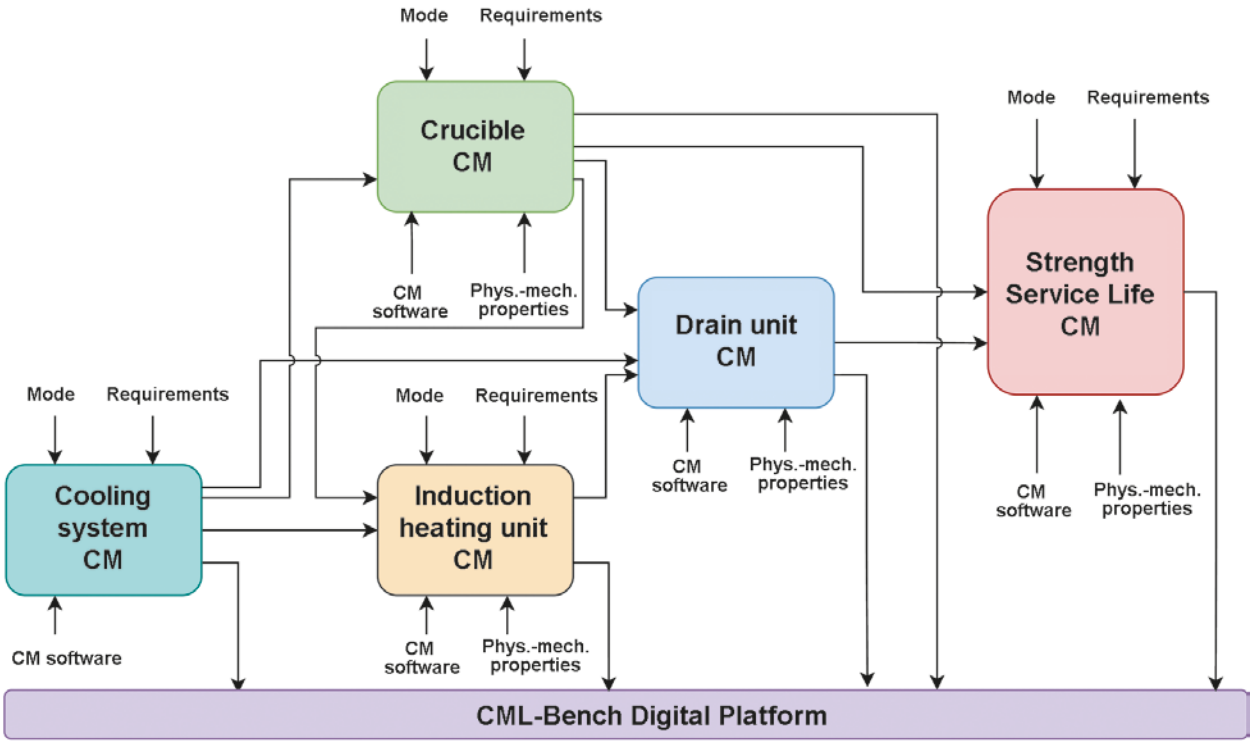


Fig. 4. Computer model interaction flowchart

itself in concentration of current near the conductor surface when the conductor is exposed to high-frequency alternating current.

The digital model (DM) of the melter is a system of interconnected mathematical and computer models describing:

- the crucible;
- the cooling systems;
- the induction heating unit;
- the drain unit;
- estimated strength and (service) life.

Fig. 4 presents a structural diagram showing the interactions between the computer models. Depending on the best available CM software, the level of detail and the degree to which physical and mechanical processes are taken into account, the CM architecture and the coordination algorithms among them can be modified. The diagram is built in the IDEF0 notation: each block is a CM (or a complex of CMs), the arrows between them show data flows, control information is indicated as arrows at the top; tools and characteristics are shown at the bottom.

A mode map accounts for the control information for all CMs: in a formalized form it provides detailed description of the product's operating modes.

When relationships between computer models are specified, some difficulties may arise due to data transfer, since different CMs are often built assuming the use of different engineering software. This problem can be addressed by automated calculation chains (actually scripts) based on which output data from one CM implemented in a certain software system can be processed and then these data can be transferred to another one implemented in another software system as input information in the form of boundary conditions. Integration links in Fig. 4 are shown by arrows.

A key task addressed by the melter accounts for effective generation of a non-stationary spatial temperature field corresponding to the required process stage:

- in the cooling mode, which may last from 8 to 12 hours, homogenization of the melt should be ensured, however the melt bottom part can't be heated to the temperature allowing the melt to discharge;
- the discharge mode is characterized by several short intervals during which the bottom part should be heated by changing the switching of the electrodes and connecting the induction heating unit followed by its disconnection and bottom part cooling to the temperature, at which the discharge stops.

The cooling system plays an important part in these processes. It must effectively manage the heat flows and maintain the required temperature, digital (virtual) testing of the cooling system allows evaluating its efficiency, i. e., sufficiency of heat removal rate for achieving the required process parameters.

The cooling system CM is a set of mathematical and computer models representing its components and units, such as peripheral cooling of the melter body, cavities of the bottom electrode, lid and drain

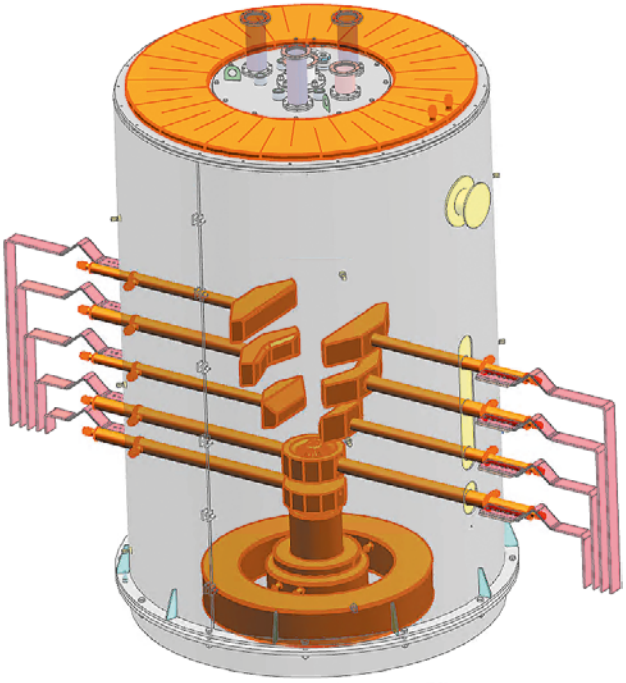


Fig. 5. Main components of the melter cooling system

outlet channel, circuits of the melter base, as well as current leads and connected air supply lines. Its main units used to build the CM are shown in Fig. 5.

In the melter CM, the operational flowchart is described by a sequence of quasi-stationary states. Digital (virtual) tests performed to explore a set of such conditions corresponding to an actual procedure may provide a data array based on which the thermal state can be evaluated, as well as data on the relationship among the convective heat transfer coefficient, temperature and air pressure for each of the system elements.

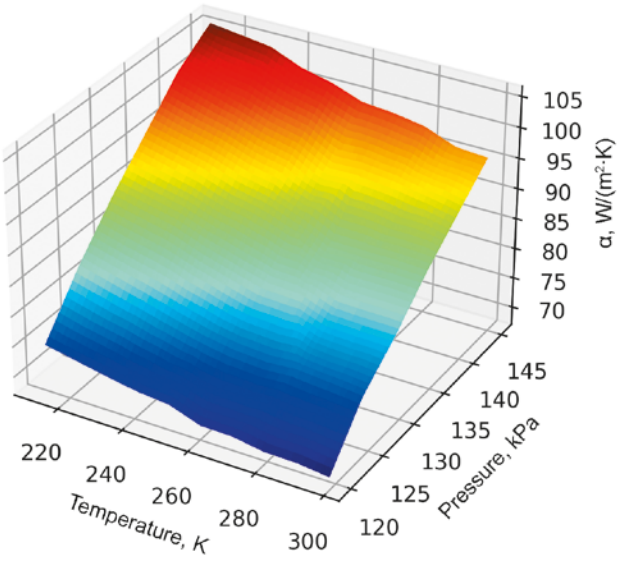


Fig. 6. Diagram showing the dependences between the convective heat transfer coefficient a on the surfaces of the cooled electrode and the air temperature and pressure in the system

The results of such digital element tests can be presented as three-dimensional diagrams. Fig. 6 shows a diagram created for one of the cooled electrodes.

Such multivariant calculations are performed in the CM software to solve continuum mechanics problems via the finite volume method, while the CML-Bench® digital platform enables flexible integration of any necessary software. Fig. 7 and 8 visualize the velocity field displaying the current flow lines in the section.

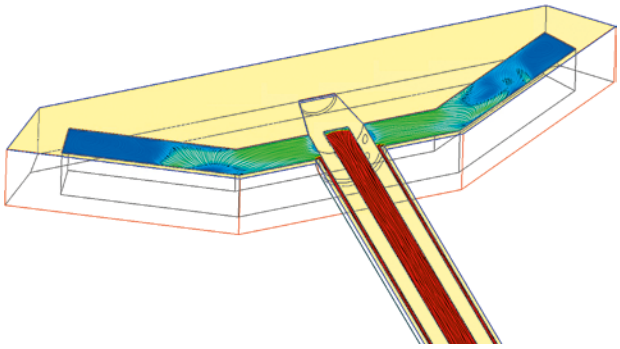


Fig. 7. Velocity field in the cross-section of the cooled electrode cavity model

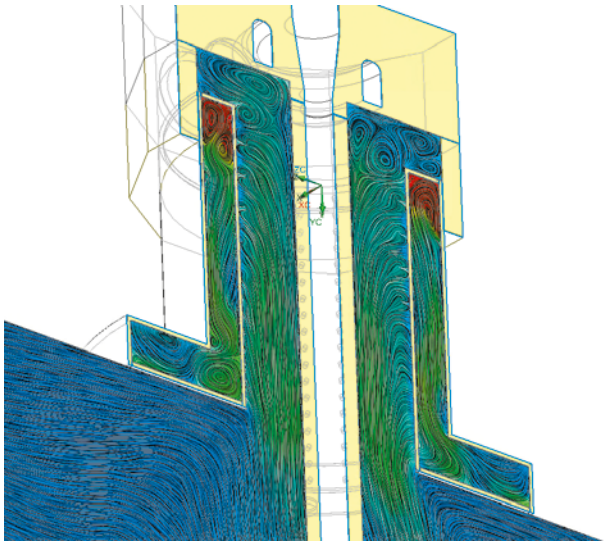


Fig. 8. Velocity field in the cross-section of the cooled drain outlet channel model

The crucible CM is a multidisciplinary CM designed to determine the thermal state in various operating modes of the industrial facility. This CM can be used to model the following physical processes in the crucible:

- electric current flow through the melt pool;
- heat exchange;
- thermal radiation from surfaces;
- convective heat transfer.

The CM provides for steady-state and transient calculations. It can be integrated with other CM elements via some additional software modules that

process computer modeling results in a format suitable for transfer.

OpenFOAM is the main software tool used for solving hydrodynamic problems in the digital model of the melter. This software tool calculates continuum mechanics problems based on the finite volume method and allows one to change the source code when the user needs to create some specific models and calculation algorithms. This software is able to simulate physical processes related to hydro- and gas dynamics, heat exchange and electromagnetism. Its key advantage is viewed in its ability of taking into account their multiphysics, which is especially important when one needs to model melt heating functions in a crucible, where electromagnetic phenomena may heavily impact relevant thermal and hydrodynamic processes.

The CM architecture is flexible enough to introduce some changes to the list of applied software, if necessary.

Digital (virtual) tests of the drain unit include computer modeling of the furnace bottom thermal state, specification of the time characteristics for the glass melt discharge processes and tests performed to elaborate the sequence of operator actions enabling the selection of optimal operating parameters for the cooling system and the induction heating unit. Thermal calculation of the glass melting and melt discharge processes was considered in [19].

In the drain unit CM, both thermal and hydrodynamic effects of the procedures initiating and discontinuing the glass melt discharge are studied. To track the melt level and model the glass melt flow correctly, multiphase flow modeling methods shall be applied. Commonly used is the free surface modeling method, which is referred to as the Volume Of Fluid (VOF) in foreign literature. Taking into account fairly high resource intensity of computer modeling, both axisymmetric and three-dimensional model can be created. To implement this feature, an additional integration module was developed: it transfers data from a three-dimensional crucible CM to an axisymmetric model of the drain unit (the bottom part of the crucible).

The drain unit CM is divided into two components: one corresponds to the initiation of the glass mass flow with initial and boundary conditions and the second one to its termination or discontinuation. The input data imported into this model include:

- the temperature field transmitted from the crucible CM describes the temperature distribution in the melter at the time immediately before the start of the discharge, i.e. taking into account reswitching of the electrodes and heating of the bottom part;
- the heat release rate along the drain outlet channel is transmitted from the induction heating unit CM to assign it as boundary conditions and provide adequate heating of the bottom part required for the start of the discharge;
- heat transfer coefficients and air temperatures corresponding to the discharge initiation and discontinuation are imported from the cooling system CM.

Based on computer modeling of the start of the discharge, data on the temperature field in the melter are saved and subsequently uploaded, which ensures a correct assignment of the initial temperature distribution in the discharge discontinuation CM. In particular, it corresponds to a set of imported data similar to the discharge initiation one, but with different values of the applied boundary conditions. These processes mainly differ by the fact that during the discharge initiation, all boundary conditions are associated with an increase in the temperature of the bottom part, and in the case of the discharge discontinuation — with a decrease in the temperature aimed at achieving partial solidification of the glass in the drain outlet channel.

The induction heating unit CM is a multidisciplinary model applied to evaluate the electromagnetic fields and the thermal state of the drain outlet channel and the inductor spiral. In the basic version, it is designed to solve an axisymmetric problem of alternating currents and, therefore, to evaluate the magnetic fields and determine the heat release rate in the drain outlet channel due to induced high-frequency currents generated by an inductor with pre-known electrical parameters (current or voltage). The resulting data are transferred to the drain unit and crucible CMs to specify the thermal state of the furnace.

CMs implemented on the digital CML-Bench® platform may be used to solve some specific problems required to establish optimal element configuration (for example, the inductor coil) or to select an adequate operating mode.

Due to the cyclical nature of industrial unit operation, computer modeling is a must when one needs to determine the number of parts and the cyclic durability of the structural elements. Strength and service life CM is designed to analyze the compliance with reliability and durability requirements in cases when thermocyclic stresses occur. The model relies on analytical relationships applied for service life assessment (Manson formula) based on finite-element evaluation of the thermostatic stress fields.

Virtual sensors (i. e. points of data collection from other CMs) are installed in the industrial unit digital twin and can be located in any structural component. Obviously, it is desirable to install them first in critical zones, as well as in areas where

actual sensors had been already installed: this is required for CM validation and to analyze the functional characteristics of the product. On the digital CML-Bench® DP platform, the virtual sensor model is a document providing information about virtual sensors and devices actually installed on the product, as well as a software program that collects and records relevant information.

For the considered melter design, analysis was performed of the data on the glass melt holding mode testing available in the Mayak PA pilot facility information system. Python language and the Pandas library were used to develop a code (script) for reading data from the analyzed sensors, visualizing information on specific time intervals and calculating time-averaged values and based on them compiling files with target values presented in an appropriate format suitable for their uploading to the CML-Bench® DP.

Model Development and Validation Results

Fig.9 presents an example of representation of temperature distribution fields in the melter under the glass melt holding mode.

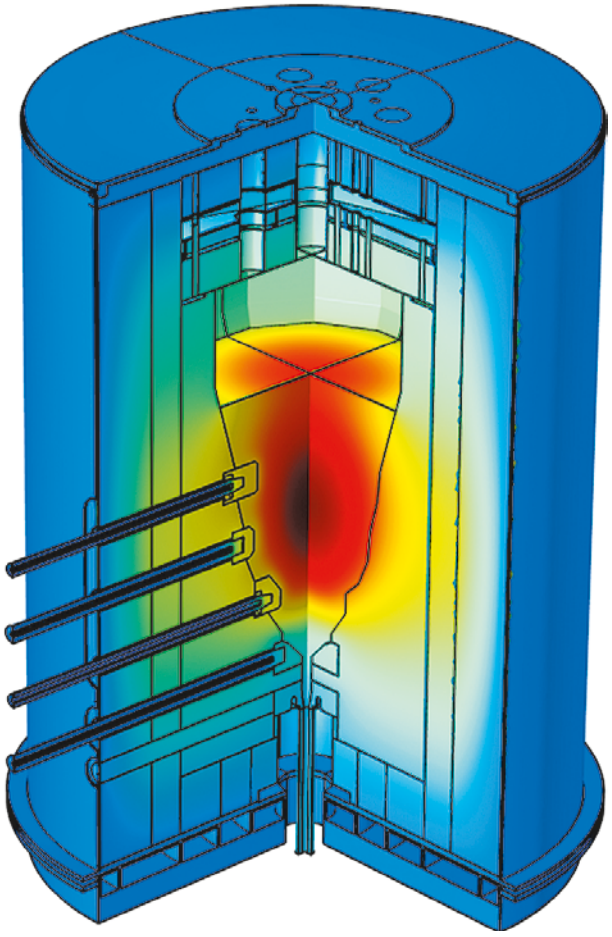


Fig. 9. Temperature fields in the melter in the glass melt holding mode

The CM relevance to a real object can be estimated using validation. For this purpose, a matrix of target parameters based on data from full-scale tests (temperature data from sensors — thermocouples) is developed. When the crucible CM was under development, certain scripts were implemented to analyze the computer modeling data on melter operation and to upload the temperature readings from the thermocouples to the CML-Bench® DP.

Comparison of the experimental data and the computer modeling results is shown in Fig. 10. On average, the differences in the key characteristics based on thermocouple readings did not exceed 10%, which can be considered satisfactory given the complexity of the physical and mechanical processes and the operational modes.

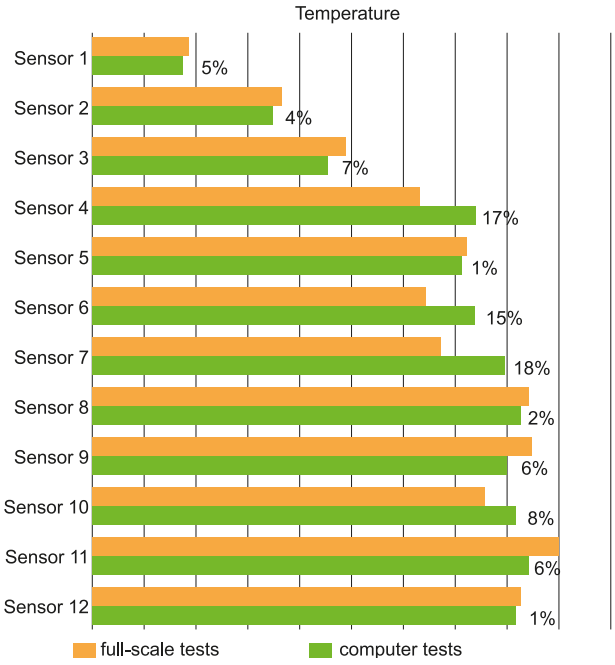


Fig. 10. Histogram comparing temperature data based on computer modeling and the data from real sensors

Conclusion

Digital Twin (DT) and virtual testing technologies allow carrying out related and multiphysics calculations and may considerably reduce the design costs of industrial facilities development and facilitate the market launch of new advanced products. Under the present study, the CM architecture was implemented for a small-sized melter, including a system of mathematical and computer models describing the operation of its main components: the crucible, the cooling system, the drain unit and the induction heating system.

Validation of the developed computer models based on data from full-scale tests showed that the discrepancy in the temperature data obtained

from real and virtual sensors accounted for no more than 10% (Fig. 10). This confirms the high level of adequacy of the developed small-sized melter CM representing a system of interconnected mathematical and computer models. To further refine and improve their adequacy level, a number of key parameters to be considered under such validation should be increased, which highlights the importance of attaining higher-quality experimental results, as well as elaborating physical and mechanical material properties and the data from the pilot melter operation.

When it comes to complex industrial equipment, digital transformation of the design development and operational processes requires an integrated information space to manage the product data (quantitative and qualitative characteristics, design documentation and many other parameters). In this context, the CML-Bench® DP helped computerize computer modeling, handle large data volumes resulted from multivariant digital tests and interconnect different computer models/

The developed CM architecture, which includes a system of related mathematical and computer models, is provided with a necessary set of tools that:

- identify the optimal operating mode for the cooling system;
- model the initiation and discontinuation of the glass melt discharge process.

The implemented melter CM is a result of successful application of the DT technology. The discussed approach applied to its architecture development can be used at various stages of the product lifecycle: to develop and improve product design parameters, to plan relevant experiments and to optimize the operational processes.

It should be emphasized that the digital twin is based n a CM, i. e., a system of complex multidisciplinary mathematical and computer models. To introduce any important changes to them, some laborious processes should to be initiated to refine the entire chain of transformations. A promising approach proposed to address this problem is viewed in the development of reduced-order models based on a full-scale DT. Simulation based on these models is of much less computational complexity and requires less CM storage capacity while maintaining a specified level of its adequacy within controlled deviations from the full-scale test results. Furthermore, at the operational stage, relevant subsystems should be maintained at an optimal level, parameters should be monitored provided that the anomalies are detected, and in some cases, detailed predictive monitoring may be required. The concept of an intelligent assistant for the studied melter was described in [22].

Thus, when it comes to multiphysics processes occurring in industrial plants of this type, a certain system of approaches and technologies may yield a sufficient degree of detail and also increase considerably the adequacy of mathematical and computer models representing a specific object and real processes. When new and advanced products are developed, it becomes necessary to systematize and digitally transform the development and design process based on the digital twin technology [5]. Thanks to this approach one may avoid a situation when the number of changes and, consequently, the higher costs associated with their introduction are distributed throughout all lifecycle stages. A large portion of changes and, thus, costs, account for the design development stage, during which competitive functional, technical and cost characteristics are shaped. These should ensure the superiority of national technologies and products over foreign counterparts, which is currently viewed as a national task for attaining the technological leadership.

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