



**Ural Federal
University**

named after the first President
of Russia B.N. Yeltsin

**Institute of Physics
And Technology**

Numerical solution of the coefficient inverse heat conduction problem to clarify the properties of non-metallic materials

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Relevance

Computer modeling of technological processes is a priority direction in the development of engineering software as part of import substitution of critical production segments in the defense industry.

- The reliability of computer modeling of temperature fields in technological processes is determined by the accuracy of the input data and the properties of the materials.
- High temperature process simulators come with a limited material database.
- The thermophysical properties of materials at high temperatures cannot always be reliably measured.
- Foundry molding materials are not standardized and quickly change their properties after preparation.

→ It is relevant to clarify the thermophysical properties in the materials database of the technological process simulator by solving the coefficient inverse heat conduction problem.

Novelty

- The Levenberg-Marquardt method used in solving the inverse problem works effectively in deep learning technologies for neural networks.
- Features of the field of application of the method require the search for effective restrictions to ensure the convergence of the algorithm.

→ The proposed approach to creating a database of simulator materials is new.

Aim of the work: to develop of an algorithm for solving the coefficient inverse heat conduction problem and implement it as a module that corrects input data for computer modeling of foundry technologies.

Objectives:

1. Perform an analysis of possible methods for solving the inverse heat conduction problem in relation to computer modeling of temperature fields and simulation of technological processes of crystallization of a metal alloy surrounded by a non-metallic material.
2. Perform an analysis of the reliability of temperature measurements with thermocouples in experiments on the crystallization of a metal alloy in a sand casting mold.



LVMFlow

modeling of foundry processes

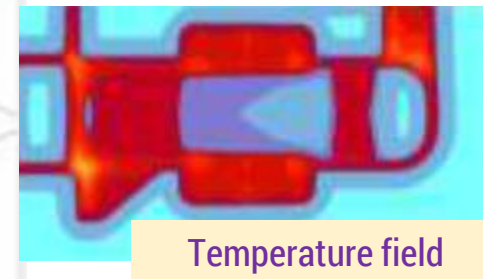
3. To develop a computational model or a full-scale experiment on the crystallization of aluminum alloy AK7ch to solve the direct heat conduction problem in the LVMFlow software environment.
4. To develop and study an algorithm for solving the inverse coefficient heat conduction problem to determine the thermophysical properties of sand mixtures from which foundry molds are made using 3D printing.
5. Implement the developed algorithm as a software module using free software.

Objectives set on real production →

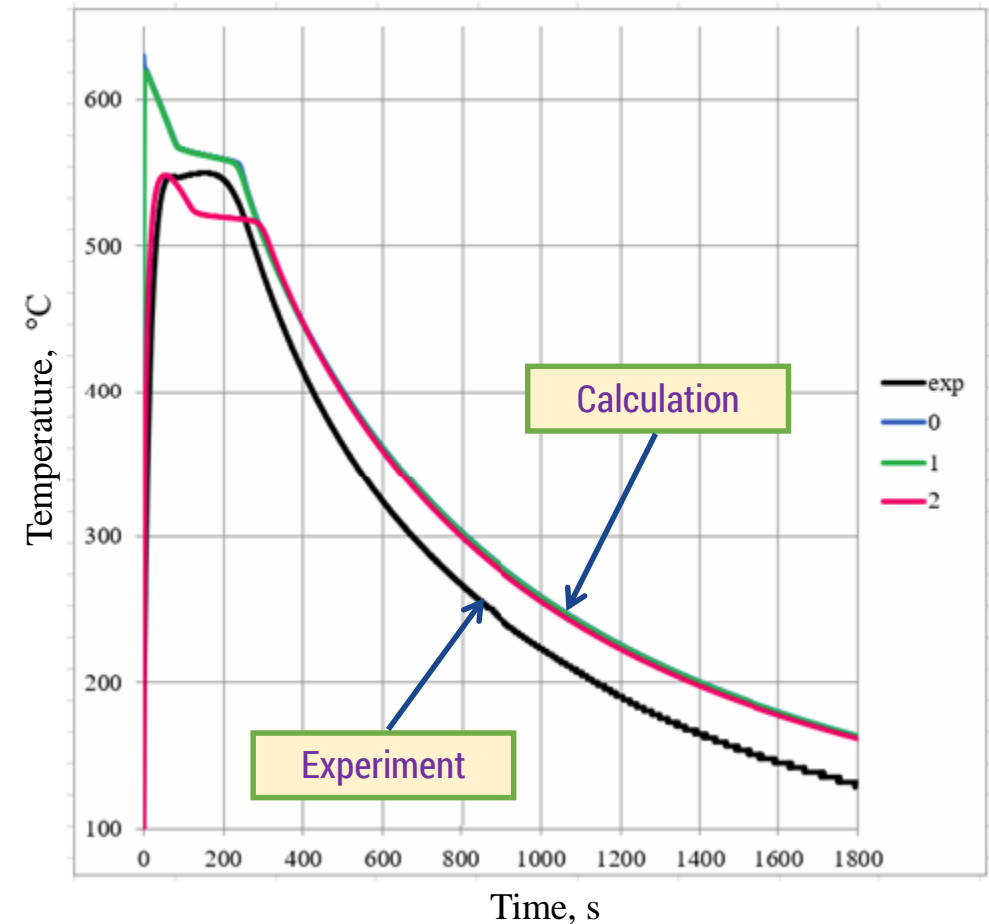
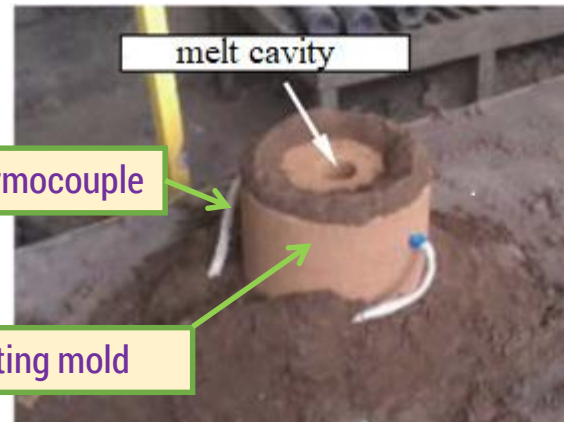
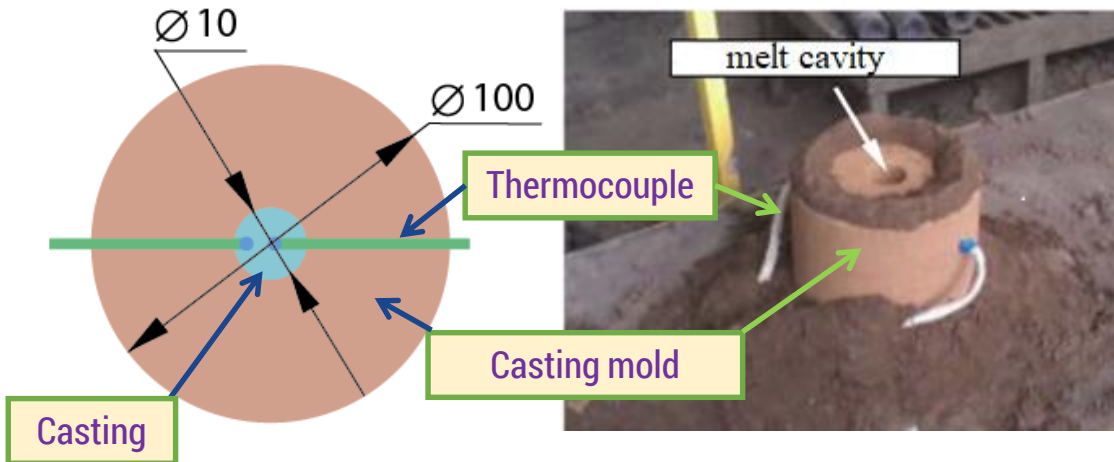
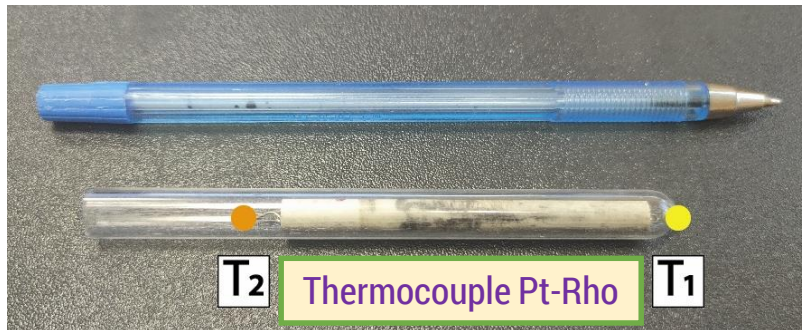
- This work was completed in accordance with the problems of high-tech digital production.
- The problems of the work concern the reliability of computer modeling of foundry technologies using new casting tools made from sand mixtures using additive methods.
- The technical specifications were initiated by specialists from the foundry equipment design bureau of JSC NPK Uralvagonzavod (Nizhny Tagil).

- The developed software module is installed and tested in the foundry equipment design bureau of JSC NPK Uralvagonzavod (Nizhny Tagil).
- This application will be submitted to Rospatent for state registration of the program for electronic computers.
- The main practical result of the research is that the thermophysical properties of the sand mixture for 3D printing of equipment at the enterprise have been clarified in the materials database of the Russian simulator LVMFlow.

→ Implementation the results in real production

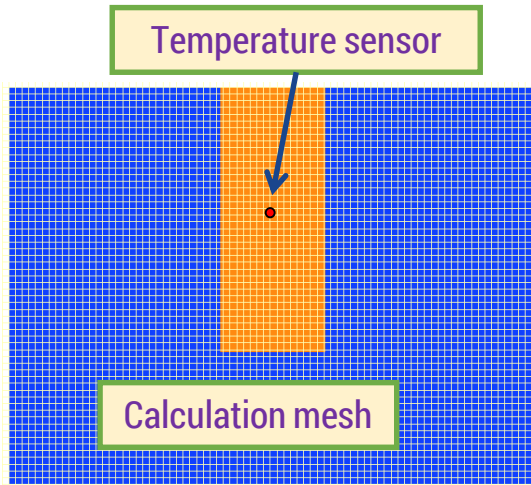
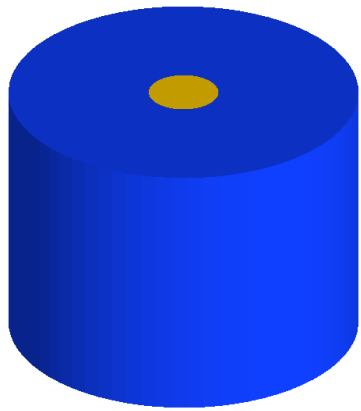


- Test experiment in factory conditions.
- Sand mold.
- Cylindrical geometry.
- Thermocouples are put down in the AK7ch melt.

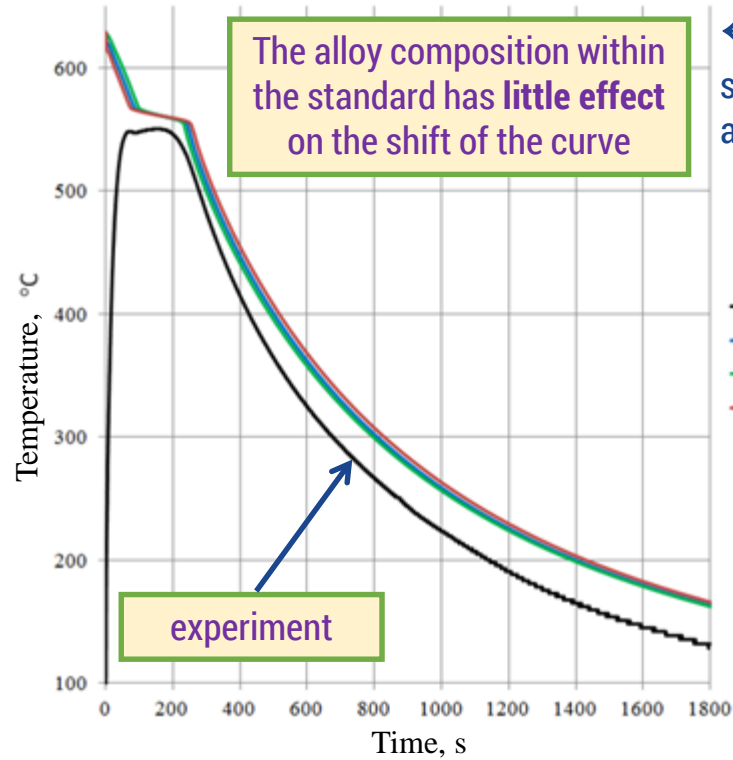


If the properties of the sand mixture are not specified accurately, the calculated temperature curves do not coincide with the experimental one.

A computational model of a full-scale experiment on the crystallization of the AK7ch alloy in a cylindrical sand mold was constructed.

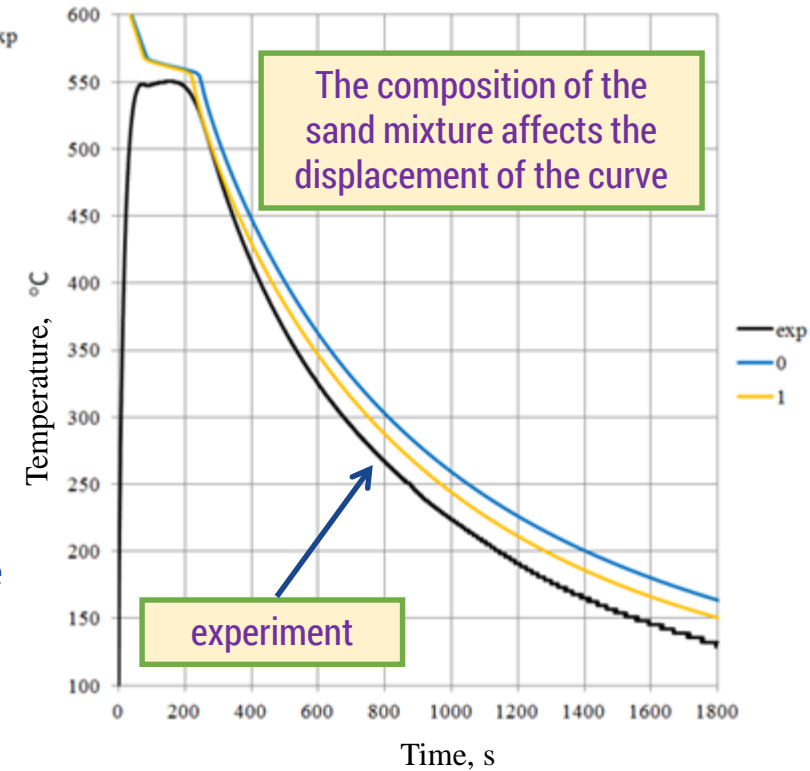


↑ Geometric model and finite-difference mesh in section with a given temperature sensor



← Temperature curves for cooling the AK7ch alloy in sand form: exp - experimental curve, calculated curves for a silicon content of 7% (0 - initial), 6% (1), 8% (2).

Temperature cooling curves of AK7ch alloy → to vary the composition of the sand mixture from which the mold is made: exp - experimental curve, options when the binder is clay (0) and resin (1)

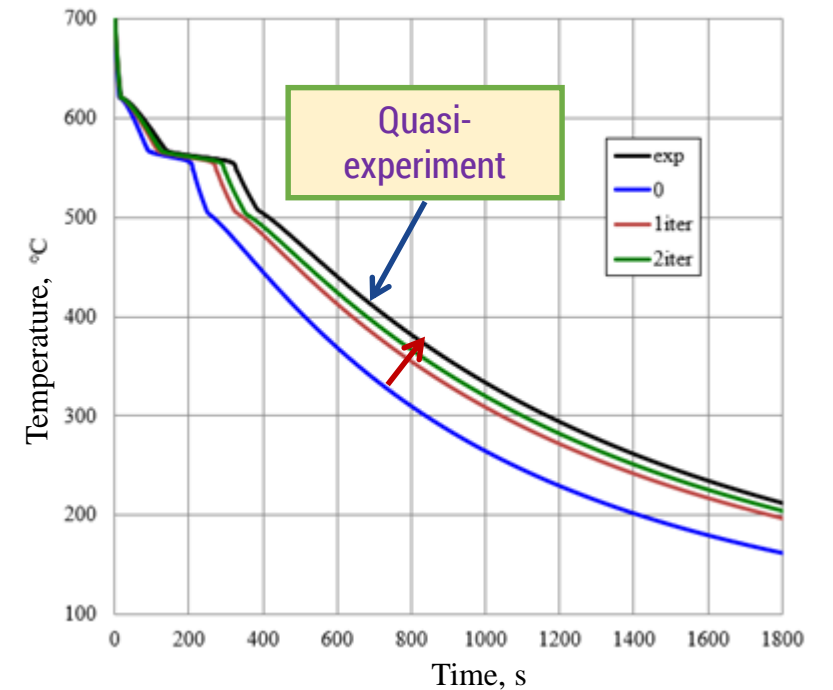
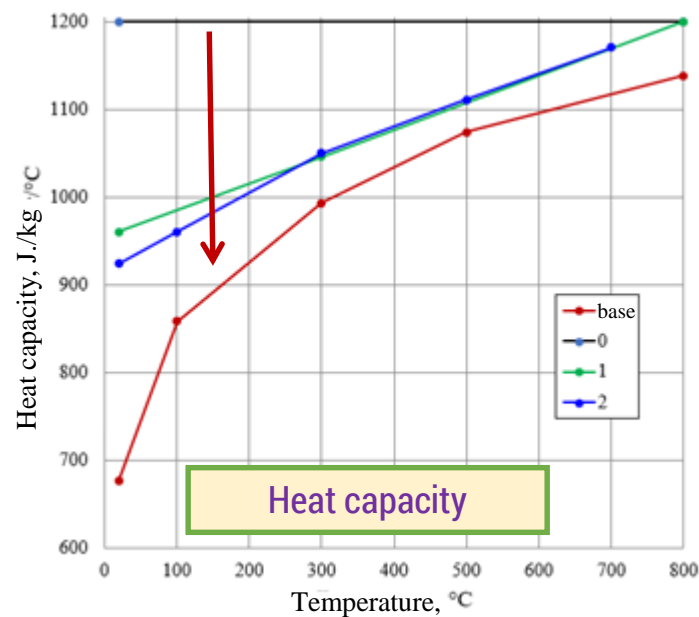
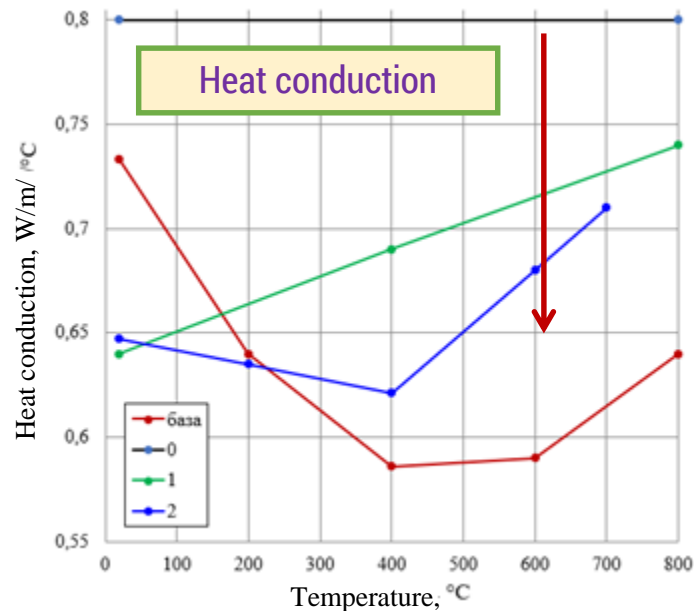


- The Levenberg-Marquardt method was chosen to solve the inverse heat conduction problem :
- The developed algorithm was implemented and studied in Scilab version 6.1.1.
- To test the algorithm, the properties of a sand-clay mixture were selected, in which quartz sand is 90%.

$$P^k = P^{k-1} + (J^T J - \mu I)^{-1} J^T (T^e - T)$$

Quasi-experimental temperature curve: a material was created in the materials database with initial values of thermal conductivity 0.8 [W/m×K] and specific heat capacity 1200 [J/kg×K] for two extreme temperature values:

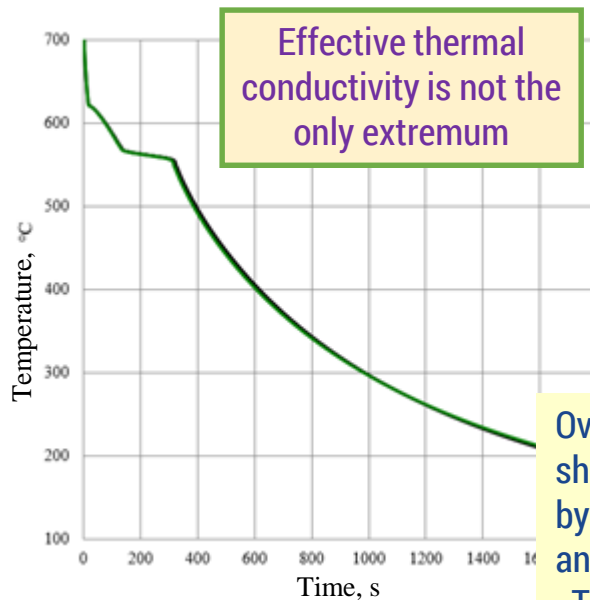
The quality factor of the calculated curve was initially 19% (curve 0), 6.9% and 3.8% after the first and second iterations (curves 1iter and 2iter, respectively):



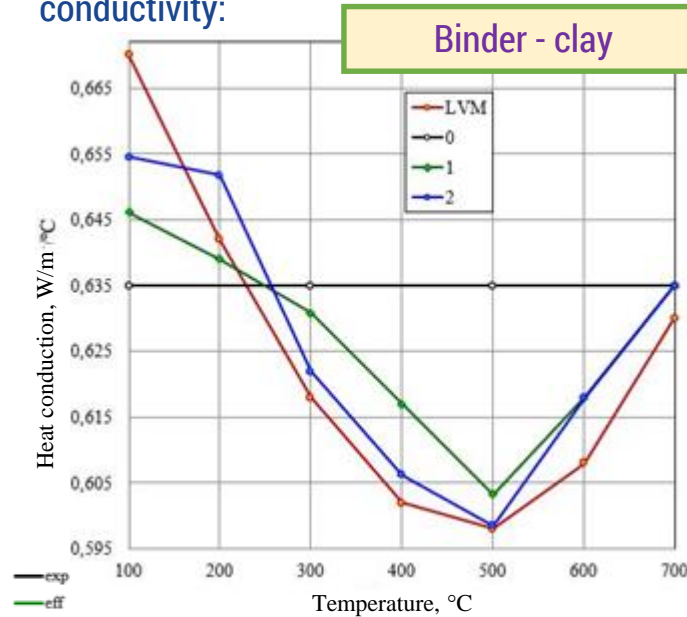
Features of the proposed algorithm:

- The algorithm uses the Levenberg-Marquardt optimization method to solve the coefficient inverse heat conduction problem.
- The algorithm generates the temperature dependence of the property, starting from one initial value, which is assigned to the two extreme points of the temperature interval.
- The algorithm is iterative and compresses the property dependence graph at each iteration, adding a new point between two existing ones according to a linear law and thus minimizing the amount of calculations.
- The algorithm checks and excludes singular points from the formation of the Jacobian matrix according to the coefficient of proximity of the temperature curve in trial computational experiments to the original calculated curve, which ensures the reversibility of the Jacobian matrix.
- The algorithm generates a square Jacobian matrix by selecting temperature curve points in an amount equal to the number of property points.

Non-single extremum problem: One effective mold thermal conductivity value of 0.635 W/m×K produces the same temperature curve as a tabular thermal conductivity function with 10 property values ranging from 20 to 800 OC:

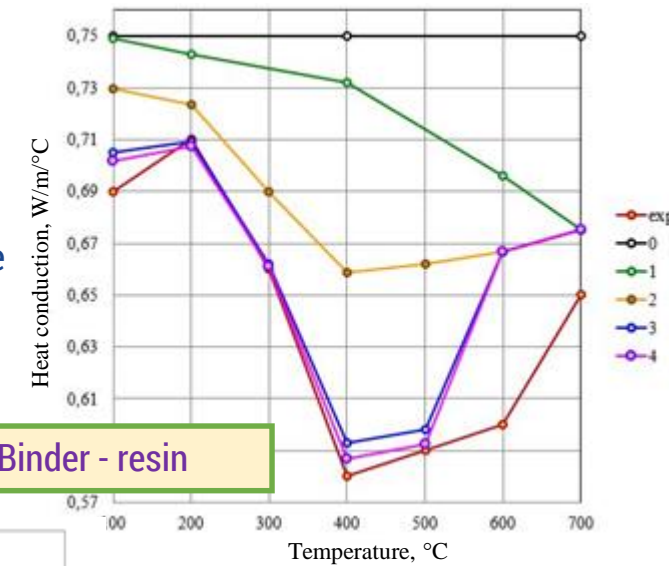
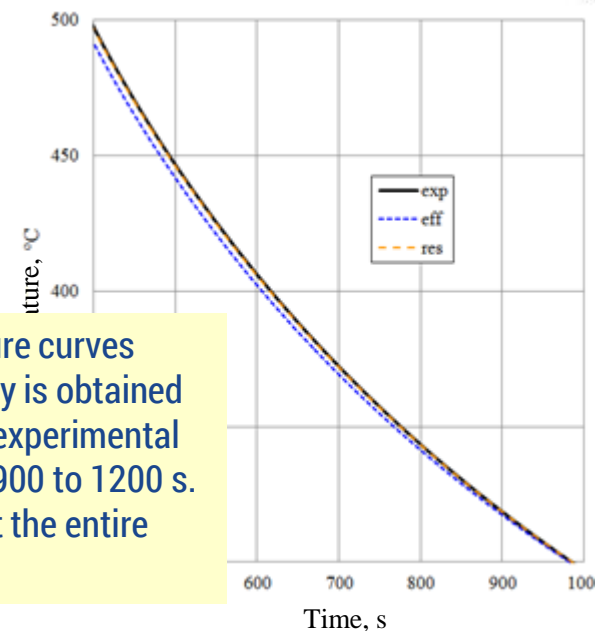


Iterations of the developed algorithm, which starts from an unstable extremum corresponding to the effective value of thermal conductivity:



Overcoming the problem: a comparison of temperature curves shows that the effective value of thermal conductivity is obtained by combining the temperature curves (conditionally experimental and calculated) in a small central time interval from 900 to 1200 s. The algorithm begins to combine curves throughout the entire time interval.

In 3D printing technologies for casting molds, sand mixtures are used, where the binder is resin. In a computational experiment, a sand mixture alpha set was selected from the LVMFlow material database:



The result of solving the inverse problem of thermal conductivity is the temperature dependences of thermal conductivity and specific heat capacity for the sand mixture, which is used in the conditions of JSC NPK Uralvagonzavod for the manufacture of technological equipment by printing on a 3D printer.

The algorithm is implemented in the SciLab software environment for further compilation into a stand-alone program in the C language.

Compilation of the Jacobian matrix based on the results of trial computational experiments, in which the displacement of the temperature curve is recorded with a small change in each point of the property vector:

Program code for changing the starting properties and calculating the properties for the next iteration (or the final property values):

```
//-----
PropConductivity = [0.8; 0.8]; // 01.
PropCapacity = [1200; 1200]; // 02.
PropConductivityScale = 1000 * PropConductivity; // 03.
PropertyInitial = [PropConductivityScale; PropCapacity] // 04.
[a1, a2] = size(PropertyInitial) // 05.
//Fill in the vector of initial calculated temperatures // 06.
TempTimeCalc = Tth(1, :, 2) // 07.
//Create a matrix of test temperatures // 08.
for f_i = 2:t_n+1 do // 09.
    TempTimeProb(:, f_i-1) = Tth(f_i, :, 2) // 10.
end // 11.
//Create a Jacobian matrix // 12.
for i = 1: 1: a1 // 13.
    J(:, i) = (TempTimeCalc - TempTimeProb(:, i)) / (0.1 * PropertyInitial(i)) // 14.
end // 15.
//Check singularity // 16.
cond(J) // 17.
cond(J'*J) // 18.
inv(J'*J) // 19.
//Enter the regularization coefficient // 20.
CoefReg = 1 / cond(J'*J) // 21.
//-----
```

```
//-----
//Suggest changes to starting properties // 01.
DeltaProp = (inv(J'*J + CoefReg * eye(J'*J)) * J') * DeltaTempExpCalc // 02.
DeltaPropProcent = diag(100 * diag(DeltaProp) // 03.
*inv(diag(PropertyInitial))) // 04.
//Normalize the change in properties by 20% // 05.
ChangeProp = 20 * DeltaPropProcent / max(abs(DeltaPropProcent)) // 06.
//Calculate property values for the next iteration // 07.
PropertyNext = PropertyReal + 0.01 * diag(diag(PropertyReal) // 08.
*diag(ChangeProp)) // 09.
disp('PropertyNext = ', PropertyNext) // 10.
//-----
```

In the development of the algorithm, it is planned to introduce an estimate of weighting coefficients for all elements of the property vector.

1. An analysis of approximate methods for solving the inverse heat conduction problem is performed and the choice of the Levenberg-Marquardt method for refining the coefficients of the nonlinear heat equation is justified. The Levenberg-Marquardt method was chosen because it does not explicitly refer to spatial coordinates when constructing the Jacobian matrix. This approach to constructing an algorithm allows us to refine models for complex geometric objects.
2. An analysis of the reliability of temperature measurements by thermocouples in experiments on the crystallization of a metal alloy in a sand casting mold was performed. For the crystallization of the AK7ch alloy in sand form in test experiments with a cylindrical sample, an interval from 300 to 1500 seconds was selected, which can be used in solving the inverse problem of thermal conductivity.
3. A computational model of a full-scale experiment on the crystallization of aluminum alloy AK7ch has been developed to solve the direct problem of thermal conductivity in the LVMFlow software environment. The thermocouple geometry has been added to the computational model of the cylindrical sample.
4. An algorithm has been developed for the numerical solution of the inverse coefficient problem of unsteady thermal conductivity to determine the thermophysical properties of sand mixtures from which foundry molds are made using 3D printing. The developed algorithm is implemented as a software module using the free SciLab software.
5. The developed software module is installed and tested in the foundry equipment design bureau of JSC NPK Uralvagonzavod (Nizhny Tagil).

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**THANK YOU FOR
ATTENTION!**