Estimation of thermal boundary conditions based on bio-inspired optimization procedures

PhD dissertation theses

by

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1. Introduction

This dissertation discusses about investigation of a numerical procedures proposed for quantitative characterization of the heat transfer phenomenon that occurs during immersion quenching of steels.

Immersion quenching of steels is one of the most commonly used heat treatment processes. Generally applied immersion quenching heat treatment of hypoeuctectoid structural steels consists of austenitizing the workpiece and its subsequent during rapid cooling. Its aim is to achieve specified properties (hardness and strengths) in a predetermined proportion of the volume of workpiece. The most critical part of workpiece quenching process is the cooling using austenitizing temperature, which decisively determines material structure and mechanical properties. The cooling capacity of coolant used for quenching process depends on physical and chemical properties of workpiece and coolant, as well as their relative flow properties. It is described by its characteristic of heat removal. It is the key to ensuring the knowledge of designability of heat treatment and final properties of the product.

In addition to the heat flux, the Heat Transfer Coefficient (HTC) parameter or function is used for the quantitative characterization of stationary heat transfer phenomena. The HTC (h $[\frac{W}{(m^2 \cdot K}]$) on surface of cooled workpiece varies through space and time. Estimation of the heat transfer coefficient is a so-called inverse heat transfer problem (Inverse Heat Conduction Process (IHCP)), belonging to scope of reverse-engineering problems. The solution is most likely a sort of solution to an optimization problem or can be originated from.

Changes of temperature distribution in a workpiece subjected to heating or cooling according to time and place can be determined by solving the Fourier equation of heat transfer, under the third type boundary condition. Since the heat transfer process taking place on surface of the workpiece is non-linear (it depends on hysical properties of the workpiece (thermal conductivity, specific heat, and so on.), the heat transfer coefficient, which depends on space and time), therefore the Fourier equation does not have a closed form solution and a numerical procedure must be used.

Objective of inverse analysis in this dissertation is to provide an iterative estimate of unknown $h(t)$ function based on temperature curve formed $1D$ axis-symmetric workpiece using chosen procedures.

2. Objective

Thermal boundary condition can be estimated by temperature field. In this case, it should be produced the cause (thermal boundary condition) from consequence (formed temperature field) by an inverse analysis. For this reason, there is no single, unique solution.

Based on mathematical point of view, the problem can be formulated as an optimization. That means a measured and calculated deviation of the time dependence of an assumed initial $h(\vec{r}, t)$ distribution of the temperature values given at certain points of workpiece must be minimized.

My research objectives were directed to the development and testing of algorithms, which suitable for solving the IHCP problem, and satisfies the following conditions:

– Developed algorithm is independent of thermal model, chemical properties, diameter of an infinitely long axis-symmetric workpiece and coolant.
– Result is heat transfer coefficient depending on time or surface temperature, as a function characterizing heat transfer between workpiece and coolant.

In this thesis I analyse 5 topics to deal the possibilities of solving the problem such as graphic processor unit -, neutral network -, bio-inspired algorithms -, and gradient-based method. I am demonstrating new sort of algorithms in order to achieve the objectives.

During the development of new algorithms presented in this thesis, my motivation was driven by the fact that, if possible, in terms of efficiency or accuracy (based on the available information), they would surpass the already existing solutions operating on a similar principles examined in this thesis.

3. Methods of investigation

The estimation of the heat transfer coefficient (optimization process) consists of the following steps:

1. Measure the cooling curves at given points of workpiece during cooling process.
2. Initial values of heat transfer coefficients are chosen randomly in searching space.
3. Calculate cooling curves.
4. Compare measured and calculated cooling curves to each other, therefore, objective function can be calculated.
5. If objective function falls outside of a specified tolerance limit, should modify values of the heat transfer coefficients based on selected optimization algorithm, and restart the calculation again using step 2.
6. If approximation is correct, final result of calculation will be selected heat transfer coefficients.

3.1. Simplified gradient-based solution

Instead of using special $h(\vec{r}, t)$ distribution assumed on surface of cylindrical workpiece, HTC coefficient was assumed a direct function of temperature on surface, it is simpler $h(T(\vec{r}, t))$ function, and based on qualitative considerations, nature of $h(T)$ function can be described with a few „shape parameters”, and could be simply modified by „tuning” its shape parameters. This restriction was a significant simplification, as a result, algorithm of search task can also be used on a lower performance computer. The classical Newton-Raphson algorithm can lead to a quick result, if assumed function statement $min\ S = 0, S : \mathbb{R}^D \mapsto \mathbb{R}$ to be optimized is really true. Through value of $\nabla S(x(1))$, make a „big jump” $\Delta x = \tilde{\alpha} \nabla S(x(1))$, so that $-S(x(1)) = \Delta x^T \nabla S(x(1))$ condition should be true, and repeat this step from new point $x(2) = x(1) + \Delta x$ starting from, and so on. The solution was a sort of „transition” between the Lagrangian Gradient Method and the Newton-Raphson algorithm, which could be adjusted based on compromise between accuracy and running time.

3.2. Increased calculation speed

Assumed cooling curves of $1D$ axis-symmetric workpiece, objective function values and parameters of neural network were calculated by a Graphical Processor Unit (GPU) applying following conditions: an Nvidia GPU card was chosen, explicit Finite Difference Method (FDM) procedure was implemented to determine the calculation of cooling curves and GPU procedure was validated by the implicit Euler method on Computer Processor Unit (CPU). During the implementation, following a compromise solution between several hard-coded (i.e. shared memory size) and selectable (i.e. grid length) parameters, a significantly faster calculation method was created than the known calculation procedures of CPU.

3.3. Approximated solution by neural network

A machine learning model was applied to estimate surface heat transfer coefficient based on calculated temperature curve in $1D$ axis-symmetric workpiece. Ability (and strength) of neural networks is to find the mapping function between any input and output. Having the right amount and quality of teaching samples during teaching neural networks is always critical. Based on GPU originated method of calculation, it was possible to run an enormous amount of simulations in a reasonable amount of time, therefore, it was possible to produce the required heat transfer function – cooling curve for teaching. The task was quite complex, since the neural network had to find non-linear relationships between a large amount of data.

3.4. Extended bio-inspired (PSO and FWA) algorithms

Bio-inspired optimization algorithms are sort of methods that are generally inspired by living beings, evolution behaviours or physical principles to solve optimization problems efficiently in multifarious areas. Based on some literature sources, the Particle Swarm Optimization (PSO) algorithm is a good option for approximation of heat transfer coefficient function. To improve prediction algorithms a new extension was developed and tested to PSO and Firworks Algorithm (FWA) algorithms, to estimate transient heat transfer coefficient function on surface of $1D$ axis-symmetric workpiece.

3.5. *Present a novel FWA approach*

A novel FWA variant for solving IHCP problems, especially for estimating $1D$ axis-symmetric workpiece of heat transfer function on surface, was produced. This new algorithm introduced completely new sparks, as well as redefined equations of motion of already known (Explosion and Gaussian) sparks, in other words, it transforms FWA algorithm on a completely new basis, while keeping their fundamentals. New calculation procedure took into account the predetermined characteristic of the time-varying heat transfer function as an optimization constraint as well.

4. New scientific results

1. A data-parallel, GPU optimized calculation procedure and a function library were designed and implemented for efficient calculation of one-dimensional axisymmetric cooling curves. Some

tests with different configurations were performed to determine parameters of the model and examine performance of the implemented functions. This method takes into account architectural possibilities and limitations of both CPUs and GPUs, applying appropriate optimization techniques to achieve the maximum possible computational speed and to increase the number of cooling curves that can be calculated in parallel for GPU. Results of practical tests proved that implemented method was significantly faster than the well-known calculation methods for CPU.

2. A suitable methodology machine learning model was developed for estimating one-dimensional heat transfer coefficient similar to those found in reality. The evaluation of results showed the implemented method fits for generating initial state of heuristics. Calculation accuracy of the model was validated by reconstructing of hypothetical heat transfer functions.
3. Novel procedures were developed for estimating transient heat transfer coefficient function on the surface of a $1D$ axisymmetric body using Particle Swarm Optimization (PSO) and Fireworks algorithms (FWA) by introducing a secondary objective function and a mapping operator. The solutions together have increased accuracy and reduced runtime compared to the same algorithms reported in literatures. The improvement was observed in the

estimation of heat transfer coefficient functions consisting of 50 and 200 points, which was confirmed through simulation studies using theoretical heat transfer function.

4. A new type of Fireworks algorithm designed specifically suited for estimating the transient heat transfer coefficient function on the surface of a 1D axisymmetric rod. The novel computational procedure takes into account the predetermined characteristics of the time-varying heat transfer function as an optimization constraint. I proposed new types of motion equations to determine the positions of each sort of sparks. Computational efficiency of the novel method was validated in the estimation of heat transfer coefficient functions with 50 and 200 points through numerical tests.
5. A simple and computationally light method was suggested to estimate the time dependence of the heat transfer coefficient along the centreline of a 1D axisymmetric body based on the measured cooling curves. This approach utilizes a numerical solution based on a combination of the classical Gradient Method and the classical Newton-Raphson algorithm using simple parametric forms for this function were introduced and showed that the problem can also be handled on an ordinary computer with a sequential program code allowing the estimation to be performed

on an ordinary low-capacity computer.

5. Perspectives and Conclusion

Results of newly developed procedures in this dissertation show that the techniques can be successfully used with appropriate additions to find a possible solution to investigated problem. Due to the complexity of task, this dissertation applied complexity reductions. Eliminating some of these applied simplifications requires further research. Following investigations might improve the results in the future:

- Answer to question why the results calculated using bio-inspired heuristic procedures FWA and PSO show a significant deviation compared to the reference curve in the values to right of peak of $h(t)$ function, while values on left points are significantly more accurate compared to values on right side.
- In case of different heuristic procedures, to examine possibility of using $h(t)$ function obtained as an estimate of a neural network as the initial value of heuristic procedures.
- Transform procedures described in this thesis to case of $2D$ axisymmetric (cylindrical) finitely long workpiece.
- The largest proportion of calculation time of heuristic algorithms is the calculation of the cooling curves, so need more further optimization of the implemented procedure in GPU.

New scientific results of this dissertation can be used not only in the design of steel immersion quenching technology, as well as in the reliable execution of quenching operations.

- Cooling long-term food storage is a well-established procedure, where the process of cooling and defrosting the food fundamentally affects the texture and freshness of the food after defrosting.
- Estimating the expected lifespan of railway tracks (in terms of potential breakage) is a condition for safe „and cheaper" train travel. Currently, the exact time of replacing the laid railway tracks can only be determined by preliminary measurements. Due to the significant cost and time required of large number of measurements required, only a fraction of them are carried out, which is why the replacement time can only be determined within broad limits, i.e. for safety reasons, the laid railway tracks need to be replaced well before end of their service life.

6. Az értekezés témakörében készült publikációk

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