CHEMICAL ENGINEERING TRANSACTIONS

VOL. 94, 2022

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš, Sandro Nižetić

ISBN 978-88-95608-93-8; **ISSN** 2283-9216

DOI: 10.3303/CET2294072

Solution to Inverse Heat Transfer Problems by Means of Soft Computing Approach and Its Comparison to the Well-Established Beck's Method

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Many engineering problems involve heat transfer with phase change and their solution often lead to challenging heat transfer problems having no direct solution. A direct solution in this respect means the determination of the thermal behaviour of a system under imposed initial and boundary conditions. The direct solution is not possible in problems where those initial and boundary conditions are unknown. In such cases, an inverse approach has to be used. However, most of the methods available for the solution of inverse heat transfer problems have been applied to heat transfer problems without the phase change. In this respect, soft computing methods seem to be a promising approach. The reason is that soft computing methods build on artificial intelligence, nature-inspired mechanisms and other principles, which enable to effectively find a sufficiently accurate solution to even very complex problems for which hard computing approach fails. In this paper, a computer heat transfer model accounting for the phase change was created and a neural network approach, which also belongs to the soft computing family, was applied to the solution of an inverse heat transfer problem. The identical problem was also solved by means of a well-established (traditional) Beck's method and the two inverse solutions were compared to each other, including the assessment of the overall computational procedure. The results showed that the approach based on neural networks was efficient and qualitatively led to similar results as in case of the Beck's method and was computationally more efficient.

1. Introduction

Heat transfer problems with phase change can be found in many engineering and industrial processes. Many such heat transfer problems involve solid to liquid (and vice versa) phase changes: melting and solidification. Some of these heat transfer problems with phase change (HTPPC) cannot be solved directly (resulting in thermal behaviour of these systems) as some of the heat transfer parameters (material properties, initial and boundary conditions) are unknown. This is the case where the solution to inverse heat transfer problems (IHTPs) is needed. Many IHTPs are very complex and their detailed phenomenological description (in terms of governing equations) is considerably difficult or even not possible altogether, and a "black box" technique has to be applied. Examples of such problems include, for example, the degradation of performance characteristics in heat exchangers (e.g. leakage and fouling), quality issues in metal casting and processing (e.g. formation of defects) and thermal characterization of phase change materials (PCMs) used for thermal energy storage (e.g. thermophysical properties dependent on the temperature, the enthalpy-temperature relationship, and the hysteretic behaviour).

The effective operation, optimal engineering design as well as the identification of issues in engineering processes and systems involving HTPPC necessitate detailed knowledge about their thermal behaviour.

Paper Received: 15 April 2022; Revised: 10 May 2022; Accepted: 23 May 2022
Please cite this article as: Klimeš L., Kamarýt P., Charvát P., Zálešák M., Pešek M., 2022, Solution to Inverse Heat Transfer Problems by Means of Soft Computing Approach and Its Comparison to the Well-Established Beck's Method, Chemical Engineering Transactions, 94, 433-438 DOI:10.3303/CET2294072

Though experimental as well as simulation techniques can be adopted for this purpose, computer modelling and numerical analyses are often preferred over the experimental approach as they are flexible, versatile, efficient, fast and comparatively cheap. If duly validated against experimental data, computer models allow gaining results having reasonable accuracy. A typical HTPPC requires a direct solution - the transient evolution of the temperature and the overall characterisation of thermal behaviour, which considerably depend on heat transfer conditions and other parameters (input data). These inputs particularly account for initial and boundary conditions and thermophysical properties. However, in many HTPPCs, a solution to the inverse problem is required. In this viewpoint, the IHTP can be viewed as a reverse procedure to the direct problem: the information about the temperature distribution and thermal behaviour is input information, while initial/boundary conditions and/or thermophysical properties are unknown, which have to be reversely identified. In this respect, Jones et al. (1995) classified the IHTPs into two groups: inverse design problems (the aim is to identify initial/boundary conditions) and inverse identification problems (the aim is to identify thermophysical properties). Many IHTPs, however, overlap both of these groups.

Several techniques were proposed to the solution of IHTPs. Beck et al. (1982) proposed an adaptive method with a sequential determination of a boundary condition. Today, this method is considered as well-known with many practical applications. The method is based on the linearization and sensitivity coefficients. The conjugate and biconjugate gradient methods represent other approaches to IHTPs. Han et al. (2019) adopted the conjugate gradient method (CGM) to the estimation of the convective boundary condition in pipes. Cuadrado et al. (2020) presented a non-iterative inverse CGM based on a digital filter method. The Levenberg-Marquardt algorithm (LMA) and derived methods were also applied to IHTPs. However, a precise determination of the sensitivity coefficient is rather difficult in practical applications with a higher dimension, transient behaviour, and nonlinearities. Oliveira et al. (2019) used the LMA for the determination of parameters of the contact resistance at the metal-mould interface in a problem including alloy solidification.

Another group of techniques suitable for the solution of IHTPs includes nature-inspired optimization methods, metaheuristics, artificial neural networks, fuzzy logic and other related techniques, which are commonly referred to as soft computing. In comparison to conventional hard computing methods, soft computing algorithms seek an approximate solution, rather than the exact one. Czél and Gróf (2012) studied a genetic algorithm (GA) in the inverse identification of temperature-dependent thermal conductivity. Mirsepahi et al. (2012) reported on a solution to an IHTP including thermal radiation, an artificial neural network (ANN) was applied and the authors demonstrated its good applicability. Wang et al. (2019) used a fuzzy inference method for the identification of defects in a thermal process. A good computational efficiency was reported. Singhal et al. (2020) investigated a comparative approach to inverse heat transfer analysis of extended surfaces. The comparison of several algorithms was presented, including nature-inspired techniques. The authors reported good performance of whale and butterfly optimization algorithms.

As for the solution of IHTP with phase change, only a rather limited number of research studies are available in this respect. Agarwala and Prabhu (2020) utilised experimental data coupled with an IHTP for the characterization of inorganic PCMs. Pan et al. (2020) reported a model for the estimation of the heat transfer coefficient on the surface of insulating packaging with PCMs with the use of an iterative method. Hafid and Lacroix (2016) investigated an inverse thickness prediction of a protective solid layer in molten material reactors and an LMA-based approach was applied to the estimation of thermophysical properties. Cascone and Perino (2015) used an evolution strategy algorithm for the characterisation of the enthalpy-temperature relationship of a PCM. Ousegui et al. (2019) applied an inverse method for the improvement of efficiency of a heat exchanger with a PCM. The inverse method was based on the use of the sensitivity coefficient and applied to a priori estimation of the flow rate through the heat exchanger.

It can be concluded from the above review that there is only limited information in the literature about the solution to IHTPs with phase change by means of soft computing methods. The most published studies focus on IHTPs without phase change and hard computing methods adopting linearization are often applied for their solution. Such methods seek an exact solution, which makes them rather rigid, less flexible, and their specific adaptation/modification is often required for a particular case. The present paper aims at filling this research gap. A computer model for HTPPC was developed, and an IHTP with phase change was then solved by means of the two methods: the Beck’s conventional method and the method based on artificial neural networks. Both the inverse solutions were compared to each other and to the direct solution, and the overall solution procedure of the two methods was addressed.

2. Materials and methods

2.1 Problem description

In this paper, the following transient heat transfer problem with phase change was considered. A rectangular two-dimensional domain having the dimensions 5 cm × 1 m was adopted, see Figure 1a. As explained below in detail and shown in Figure 1b, material properties corresponding to paraffin-based PCMs applicable to latent heat thermal energy storage were used in simulations. Under these considerations, the presented problem can be considered as a thin PCM layer embedded in the wall structure. Such application has attracted a lot of researchers' attention; see e.g. a study reported by Al-Absi et al. (2022) who investigated the thermal performance of wall panels incorporating a PCM and the configuration with the optimal performance was identified. As for the boundary conditions, the left-hand side of the domain was exposed to the time-dependent heat flux $\dot{q}_L$ (the Neumann boundary condition), while the right-hand side of the domain was assumed at the constant temperature T_R (the Dirichlet boundary condition), see Figure 1a. Such conditions can be viewed as solar radiation outside and the nearly constant air temperature inside the building. The top and the bottom sides were assumed adiabatic, i.e. thermally insulated.

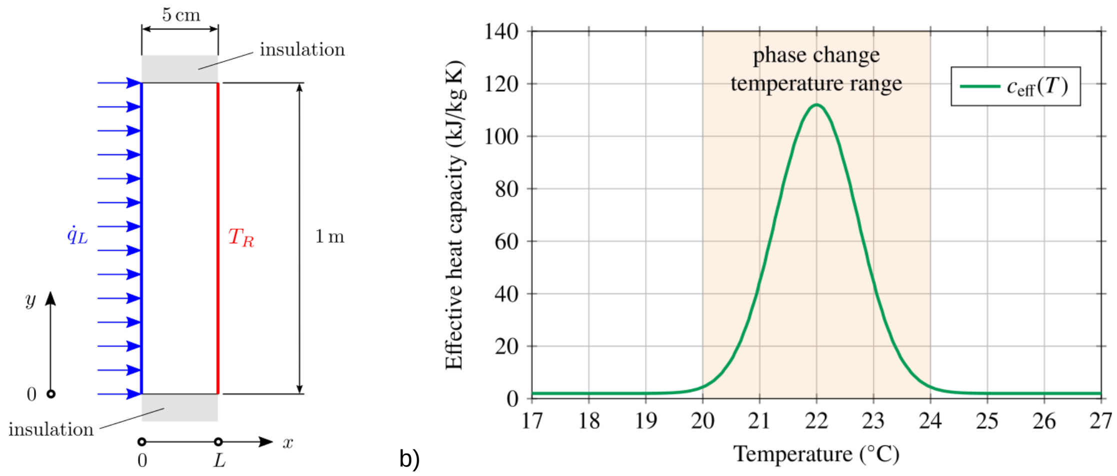

Figure 1: a) Schematic of the domain and boundary conditions; b) effective heat capacity function

As for the mathematical modelling of the presented heat transfer problem with phase change, the governing heat transfer equation describing heat transfer inside the domain and adopting the effective heat capacity for phase change modelling is

$$\rho c_{\text{eff}} \frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) \tag{1}$$

where ρ is the density of the PCM (assumed 730 kg/m^3), c_{eff} is the effective heat capacity having the bell-shape function

$$c_{\text{eff}}(T) = 2 + 110 \cdot \exp\left\{-\frac{(T - T_{\text{mpc}})^2}{1.05}\right\} \tag{2}$$

shown in Figure 1b, k is the thermal conductivity (assumed 0.2 W/(m·K)), T is the temperature, t is time, and x, y are the spatial coordinates. The mean phase change temperature T_{mpc} was set to 22 °C and the definition of the effective heat capacity function given in Eq. (2) results in the phase change temperature range of about 4 °C, from about 20 °C to about 24 °C. The boundary conditions on the left-hand side, top side, and bottom side adhere the Neumann formulation accounting for the heat flux as

$$-k\frac{\partial T}{\partial n} = \dot{q} \tag{3}$$

where the heat flux $\dot{q}$ is equal to $\dot{q}_L(t)$ on the left-hand side boundary while is equal to zero on the top and bottom sides, representing the insulated (adiabatic) walls. The right-hand side adopted the Dirichlet condition with the prescribed surface temperature, $T(L, y, t) = T_R$. Last information, which makes the mathematical formulation complete, unique and ready to be solved, is the initial condition $T(x, y, 0) = T_0$ providing the initial temperature distribution; T_0 was set to 10 °C.

2.2 Inverse identification problem

In the foregoing Section 2.1, the overall description of the considered problem was provided. In case the direct heat transfer problem is solved, the initial temperature T_0 and both the boundary conditions $\dot{q}_L$ and T_R are known and the solution to the problem means the determination of the transient temperature distribution inside the domain $T(x,y,t)$. This paper, however, focuses on the reverse process, which is referred to as the inverse heat transfer problem. In contrast to the direct problem, some of the initial or boundary conditions are unknown in the inverse problem while the response of the system – the thermal behaviour in the form of transient temperature distribution $T(x,y,t)$ inside the domain – is known. Hence, the solution to the inverse problem is to reversely determine the initial/boundary condition from the known temperature distribution, resulting into the prescribed thermal behaviour. In the present paper, a soft computing method – artificial neural networks – was applied to the solution of the inverse heat transfer problem described in Section 2.1 and further specified in Section 3. As the main objective was to address and compare the efficiency and applicability of this approach, a well-known and often-adopted sequential Beck's algorithm was also implemented for the comparison.

2.3 Artificial neural network

Artificial neural network (ANN) is a computational framework applicable to modelling and reproduction of the behaviour of complex systems or processes. The concept of ANNs is inspired by the nature – by biological neural networks, which form brains of humans and animals. The ANN consists of a set of artificial neurons, which are connected to each other and can transmit signals to each other as well. Each connection between the two neurons is quantified by a weight factor. Neurons are usually grouped into layers. A fundamental procedure is that a neuron receives a certain signal, processes it, and transmits the result to other neurons. The ANNs have a number of various applications, ranging from identification and control of systems, to pattern recognition, to data mining. The present paper does not repeat a detailed description and discussion on the principle and implementation of ANNs as there are many sources in this respect available in the current literature. The reader interested in details is therefore referred e.g. to a textbook by Aggarwal (2018), which provides comprehensive information about theory and implementation of ANNs.

A typical first phase in the use of ANN is its training, often referred to as learning: an ANN learns the behaviour of the modelled system by means of training samples, which are pairs of input and output values. During this process, the weights between the neurons are determined so that the difference between actual outputs of the ANN to the given inputs and outputs from learning samples is minimised. In the second phase, the set of weights is kept constant, and the ANN is used to predict the output to the given input values. In terms of the considered inverse heat transfer problem, the training data (samples) are pairs of initial/boundary conditions (inputs) and corresponding transient temperature distributions (outputs) from a direct model. Once a sufficient amount of training data is provided and the ANN is trained, the ANN can be used for the replication. This means that the ANN receives an input – the transient temperature distribution – and the ANN provides the output, which is the estimation of the initial/boundary conditions to the given input. The ANN procedure can be formulated as follows: (1) input data pre-processing, (2) generation of learning data, (3) ANN setup, (4) ANN learning, (5) ANN gives a prediction.

2.4 Beck's sequential method

The Beck's sequential method is based on the estimation approach to IHTPs: the unknown function describing initial/boundary conditions is assumed in a certain form of a mathematical function. Such function is further parameterised by a set of parameters and during the solution procedure, these parameters are identified. Beck et al. (1982) proposed their method on the assumption that the unknown function is seek in the form of a piece-wise constant function (each piece corresponds to a time step), and the parameters characterising the function for a particular problem are identified sequentially, one-by-one. For one so-called temperature sensor, the main task is therefore the minimisation of the error function

$$E_j = \sum_{i=1}^{r} \left(Y_{j+i-1} - T_{j+i-1}\right)^2 \tag{4}$$

where E_j is the error function for the j-th time step, r is a suitable integer parameter influencing the stability of the method (usually, r is set to three or four), Y is the known temperature in a particular location with the temperature sensor, and T is the temperature determined by the solution of the direct heat transfer model of the system. Apparently, the evaluation of the E_j function is computationally demanding, since the solution of the direct heat transfer problem over r time steps is required. Moreover, the objective is the minimisation of the function in Eq. (4), which means that a suitable algorithm is needed. Since information about the derivatives of the unknown function is not available a priori, derivative-free minimisation methods, such as the Nelder-Mead algorithm, have to be adopted. The Beck's method can be formulated as follows: (1) input data pre-processing, (2) for $i = 1$ to r do: (i) solve the direct problem for the temperature, (ii) minimise Eq. (4) to determine $\dot{q}_L$.

3. Results and discussion

The numerical model for the direct heat transfer problem with phase change described in Section 2.1 was created with the use of the finite element method and a trapezoid-based approach was applied to the time discretization. There were 297 spatial nodes and the time step was set to 0.2 s. The simulation time was set to 10 s. Two cases of the time-dependent boundary condition on the left-hand side of the domain – the heat flux $\dot{q}_L$ – were considered. One scenario (referred to as case A, see Figure 2a) assumed a discontinuous piece-wise constant variation of the heat flux while the another scenario (referred to as case B, see Figure 2b) modelled a continuous triangular-shaped variation of the heat flux. Figure 2 shows the results to the considered inverse heat transfer problem with phase change in both scenarios.

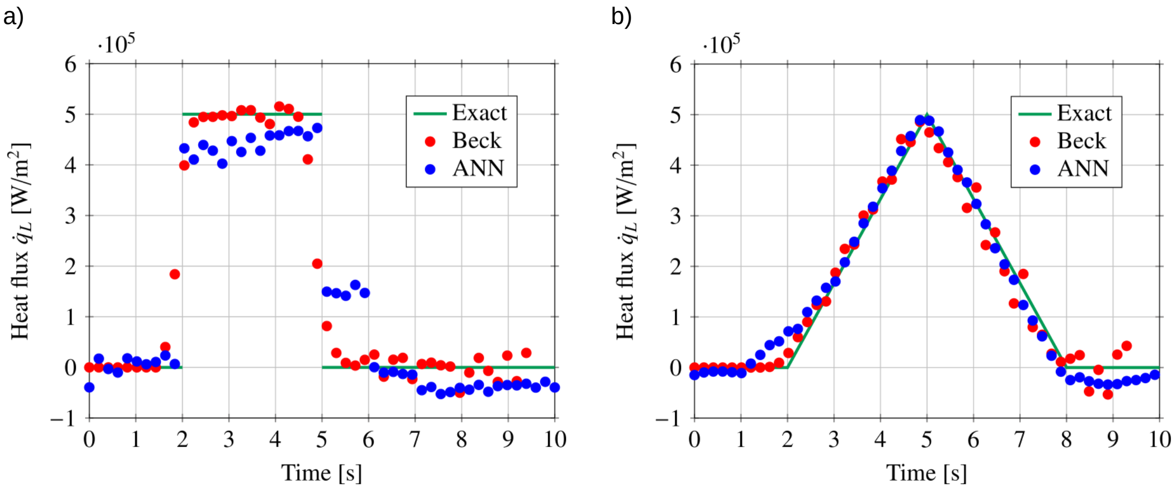

Figure 2: Results for a) the discontinuous piece-wise constant heat flux, b) continuous triangular heat flux

As can be seen in Figure 2, the ANN and the Beck's method led in both the solved cases to similar results – estimations of the heat flux $\dot{q}_L$ on the left-hand side boundary. Apparently, in case A there are more discrepancies between the exact dependence and both inversely determined estimations by the ANN and by the Beck's method. The reason for such behavior is particularly the discontinuity; many numerical algorithms suffer from low accuracy and instability in regions where the behavior is not continuous. In the second case B with the triangular-shaped heat flux dependence, the discrepancies are much lower, resulting in an overall very good inverse identification of $\dot{q}_L$ by both the ANN and the Beck's method.
As for the quantification of the quality of inverse procedure, a scaled mean square error can be evaluated:

$$\mathrm{SMSE} = (10^9/n)\sum_{i=1}^{n}(\dot{q}_{L,i} - \dot{q}^*_{L,i})^2 \tag{5}$$

where $\dot{q}_{L,i}$ is an inversely identified heat flux at the time instance i, $\dot{q}^*_{L,i}$ is the exact value of the heat flux at the time instance i, and n is the total number of time instances. The lower the SMSE is, the better the inverse identification was achieved. In the case A (Figure 2a), the SMSE equals $3.91\ \mathrm{W}^2/\mathrm{m}^4$ for the ANN and $3.36\ \mathrm{W}^2/\mathrm{m}^4$ for the Beck's method. As for case B (Figure 2b), the SMSE is equal to $0.58\ \mathrm{W}^2/\mathrm{m}^4$ for the ANN and $0.66\ \mathrm{W}^2/\mathrm{m}^4$ for the Beck's method. It can be concluded from these values that both the methods are comparable in terms of the SMSE: the Beck's method was slightly better over the ANN in case A while the opposite conclusion was observed in case B.
Besides the evaluation of the SMSE, the following pros and cons should be taken into consideration. The Beck's method: its setup is rather a trial-and-error procedure, and in particular, it is computationally very demanding (about 5 hours for the considered cases with a CPU Intel Core i5 2.5 GHz and 8 GB RAM). As for the ANN: an estimation of the unknown function can make the process more efficient. Further, the ANN is computationally rather efficient; about 30 minutes needed for training and then just a few seconds for the actual inverse identification in the considered cases.

4. Conclusions

The inverse solution to a heat transfer problem with phase change was studied by the traditional Beck's sequential method and by the artificial neural network (ANN), which belongs to the class of soft computing method. A 2D problem was considered, for which a numerical FEM-based model was developed for the direct solution. Two cases of the inverse problem were studied; case A with a piece-wise constant heat flux on the boundary of the domain while case B simulated a continuous triangular-based heat flux on the boundary. The results for the inverse problem showed that both the methods led to qualitatively comparable estimations of the unknown heat flux. In case A, the Beck's method slightly outperformed the ANN (the scaled mean square errors were $3.36\ \mathrm{W^2/m^4}$ and $3.91\ \mathrm{W^2/m^4}$, respectively), while in case B the ANN slightly outperformed the Beck's method ($0.58\ \mathrm{W^2/m^4}$ vs. $0.66\ \mathrm{W^2/m^4}$, respectively). However, the Beck's method turned out to be rather computationally expensive, while the ANN was computationally much more efficient.

Acknowledgments

This work was supported by the project Adaptive Soft Computing Framework for Inverse Heat Transfer Problems with Phase Change, reg. no. 22-31173S funded by the Czech Science Foundation, by the project Sustainable Process Integration Laboratory – SPIL, No. CZ.02.1.01/0.0/0.0/15_003/0000456, funded by European Research Development Fund, and by the project Computer Simulations for Effective Low-Emission Energy Engineering, reg. no. CZ.02.1.01/0.0/0.0/16_026/0008392 funded by Operational Programme Research, Development and Education, Czech Republic.

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