JOURNAL OF THEORETICAL
AND APPLIED MECHANICS
47, 3, pp. 701-716, Warsaw 2009

COMPARISON OF OPTIMIZATION ALGORITHMS FOR INVERSE FEA OF HEAT AND MASS TRANSPORT IN BIOMATERIALS

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Inverse analysis has become increasingly important for estimating coefficient values for heat and moisture transport in complex biological materials. With this approach, an improved accuracy of predicting transport processes can be obtained as compared to simulations based on coefficients determined by experimental procedures only. Such improvement is indispensable for successful analyzing, designing and managing most technological processes in the agri-food and forest products industries. In recent years, many optimization algorithms have been developed to solve inverse problems. Performance of the following algorithms was analyzed and compared in this paper: simulated annealing, tabu search, genetic algorithm, variable metric algorithm and trust region algorithm. Results demonstrated that although all the algorithms were able to estimate the coefficients, there were differences in their performance and due to high computational complexity of the problem only the trust region procedure was acceptable.

Key words: heat conduction, water diffusion, inverse modeling

Notations

c [J/(kg·K)]	–	specific heat
D_m [m^2/s]	–	moisture transport coefficient
D_{mt} [m^2·K/s]	–	moisture thermodiffusion coefficient

h_{cm} [m^2/s]	–	convective moisture transfer coefficient in boundary layer of domain Ω
h_{ct} [W/(m^2·K)]	–	convective heat transfer coefficient in boundary layer of domain Ω
k [W/(m·K)]	–	thermal conductivity
M [kg/kg]	–	moisture content at point $\boldsymbol{x} \in \Omega$ and time $\tau \in (0, \tau_F]$ (dry basis)
M_0 [kg/kg]	–	moisture content at point $\boldsymbol{x} \in \Omega$ and time $\tau = 0$ (dry basis)
M_e [kg/kg]	–	equilibrium moisture content determined either at point $\boldsymbol{x} \in \partial\Omega$ or at points outside boundary layer of domain Ω at time $\tau \in (0, \tau_F]$ (dry basis)
$\boldsymbol{n}$	–	unit vector normal to surface $\partial\Omega$, directed outward
t [°C]	–	temperature at point $\boldsymbol{x} \in \Omega$ and time $\tau \in (0, \tau_F]$
t_0 [°C]	–	temperature at point $\boldsymbol{x} \in \Omega$ and time $\tau = 0$
t_∞ [°C]	–	temperature at points outside boundary layer of Ω at time $\tau \in (0, \tau_F]$
t_s [°C]	–	temperature at point $\boldsymbol{x} \in \partial\Omega$ and time $\tau \in (0, \tau_F]$
$\boldsymbol{x}$ [m]	–	coordinates of point in orthocartesian system of coordinates
α_v [K]	–	coefficient used in Eq. (2.1)
ρ [kg/m^3]	–	density
τ [s]	–	time
τ_F [s]	–	instant limiting process time from right side
Ω [m^3]	–	domain of body examined in three-dimensional euclidean space
$\partial\Omega$ [m^2]	–	boundary of domain Ω ($\partial\Omega^{\mathrm{I}}$ for essential boundary condition, and $\partial\Omega^{\mathrm{III}}$ for natural boundary conditions)
∇	–	gradient operator.

1. Introduction

Biological materials are subject to intensive thermo-mechanical operations. Better understanding of heat and mass transport in complex biomaterials is an essential ingredient in the advancement of agri-food and wood processing technologies. A substantial amount of research has been focused on the development of heat and mass transport models for biological materials, and the finite element method has been the most common technique used for the numerical analysis (Irudayaraj and Wu, 1999; Weres and Jayas, 1994; Weres, 1997). However, dubious or even unknown values of biomaterial properties represented in mathematical model coefficients, often unavailable in physical experiments, restrict the usability of mathematical models. The inverse modeling approach, based on combining procedures for acquiring available experimental data, solving direct problems, computing and minimizing an objective function with the appropriate optimization algorithm, can be very efficient in estimating coefficient values of acceptable accuracy.

The objective of this study was to develop a software module for assessing performance of optimization algorithms as a part of an information system developed by the authors for inverse finite element analysis, and to compare selected algorithms with respect to bound constrained optimization for heat and mass transport in biological materials.

2. Inverse finite element approach to heat and mass transport in biomaterials

2.1. Formulation of the problem

The mathematical structural model of heat and mass transport in biomaterials, i.e. the mathematical model describing the structure of the investigated process can be represented as the system of quasi-linear differential equations of heat conduction and water transfer with initial and boundary conditions of any kind (Pabis *et al.*, 1998; Perré and Turner, 2007; Weres *et al.*, 2000):
— for $(\boldsymbol{x},\tau) \in \Omega \times (0,\tau_F]$

$$\begin{aligned} &\frac{\partial t}{\partial \tau} - \nabla\Big(\frac{k}{\rho c}\nabla t\Big) - \alpha_v \frac{\partial M}{\partial \tau} = 0 \\ &\frac{\partial M}{\partial \tau} - \nabla(D_m \nabla M) - \nabla(D_{mt}\nabla t) = 0 \end{aligned} \tag{2.1}$$

— for $(\boldsymbol{x}) \in \Omega$

$$t(\boldsymbol{x},0) = t_0(\boldsymbol{x}) \qquad\qquad M(\boldsymbol{x},0) = M_0(\boldsymbol{x}) \tag{2.2}$$

— for $(\boldsymbol{x},\tau) \in \partial\Omega^{\mathrm{I}} \times (0,\tau_F]$

$$t(\boldsymbol{x},\tau) = t_s(\boldsymbol{x}) \qquad\qquad M(\boldsymbol{x},\tau) = M_e(\boldsymbol{x}) \tag{2.3}$$

— for $(\boldsymbol{x},\tau) \in \partial\Omega^{\mathrm{III}} \times (0,\tau_F]$

$$k\boldsymbol{n}\nabla t + h_{ct}(t - t_\infty) = 0 \qquad\qquad D_m\boldsymbol{n}\nabla M + h_{cm}(M - M_e) = 0 \tag{2.4}$$

The operational form of the model was developed by the finite element approximation with the use of isoparametric, curvilinear, three-dimensional elements and recurrence schemes (two-point and three-point algorithms) in time, absolutely stable, with an iterative procedure to deal with the quasi-linearity of equations. The finite element model was enhanced with procedures controlling accuracy, stability, susceptibility to oscillations, and computational efficiency (Weres *et al.*, 2000; Weres and Olek, 2005). The final operational model for solving direct problems was composed of the two- or three-point recurrence scheme of algebraic equations, a set of data representing conditions of the investigated process, and empirical equations to calculate the equilibrium moisture content and the moisture diffusion coefficient for selected biomaterials. Numerical description of non-homogeneity and geometric irregularity of the investigated products was taken from image analysis data (Weres *et al.*, 2007; Weres, 2008).

The inverse finite element modeling procedure was based on the inverse problem approach (Isakov, 1998; Kirsch, 1996), optimization methods (Bazaraa *et al.*, 2006; Jongen *et al.*, 2004; Nash and Sofer, 1996; Nocedal and Wright, 2006; Vanderplaats, 2001), and the operational finite element model for solving direct problems described in the previous Section. Several optimization algorithms were selected and analyzed to assess their performance in minimizing the objective function with respect to the coefficients to be estimated. The objective function was defined as the L2-norm of the weighted residuals of the measured and predicted values of the quantities depicting behavior of a given biological material investigated: the temperature, moisture content, and additionally air pressure in the case of gas permeability determination (Weres and Olek, 2005; Olek *et al.*, 2003, 2005; Olek and Weres, 2005, 2007).

The developed procedure is capable of solving transient, three-dimensional, quasi-linear, inverse problems of heat and mass transport in non-homogeneous and anisotropic biomaterials of irregular geometry, with initial and boundary conditions of any kind.

2.2. Software supporting inverse finite element analysis

A software module for assessing performance of optimization algorithms (Fig. 1) was designed and implemented in Visual Studio 2008 as a part of the existing original computational and visualization software developed by the authors for inverse and direct finite element analysis (Weres *et al.*, 2007; Weres, 2008).

2.3. Optimization in constructing empirical equations

Construction of empirical equations presented in Fig. 1 was necessary to represent experimental data in a generalized form, as the input to the inverse finite element procedure of estimating coefficients of the operational structural model. Selected empirical equations were fitted to experimental data sets using the developed software (Fig. 1). The coefficient estimation for the empirical

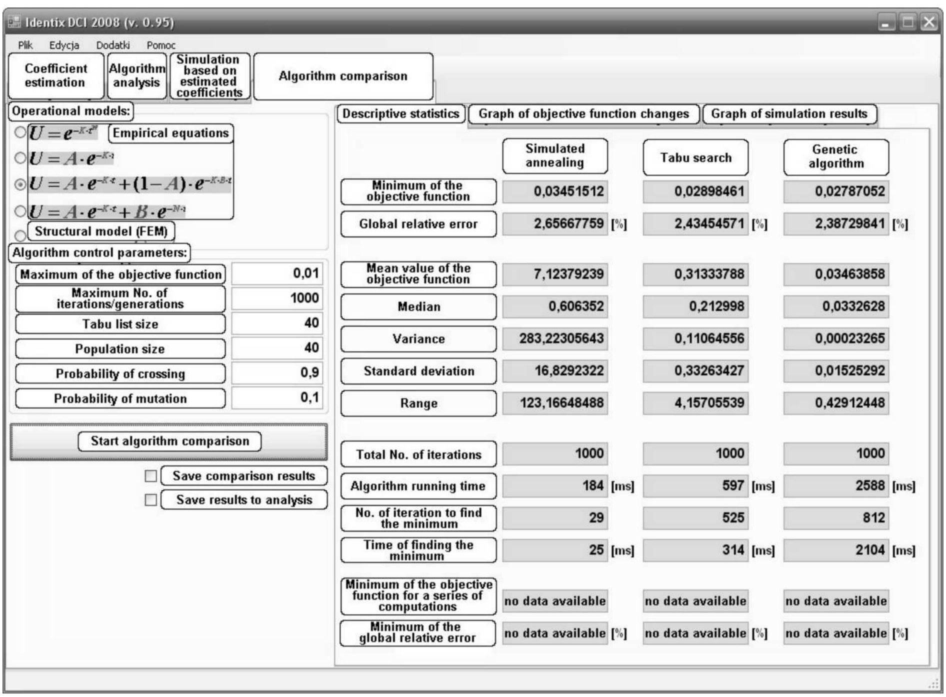

Fig. 1. An interface of the software module for assessing performance of optimization algorithms

equations was carried out with the support of the following metaheuristics designed and coded as a part of our software: simulated annealing (Privault and Herault, 1998), tabu search (Caserta and Márquez Uribe, 2009; Glover and Laguna, 1997) and genetic algorithm (Chainate *et al.*, 2007; Mousavi *et al.*, 2008), and the performance of the corresponding algorithms was compared.

To exemplify the procedure of constructing empirical equations, the water transport in corn kernels dried in thin layers was analyzed, and the resulting equations were the input to the estimation of the water diffusion coefficient, dependent on temperature and moisture content, crucial for the operational finite element model.

Details of the exemplary instance

Species: corn kernels – Clarica (FAO 280).
Drying air parameters: temperature 40°C, relative humidity 50%.
Time of drying: 24 hours.
Initial moisture content: $0.4272\,\mathrm{kg}_{\mathrm{water}}/\mathrm{kg}_{\mathrm{d.m.}}$.

Number of estimated coefficients in the empirical equation: 3.

Optimization algorithm: simulated annealing

Total number of iterations: 1000.
Initial values of coefficients: $A = 0.853368$, $B = 0.097342$, $K = 0.115924$.
Corresponding value of the objective function: 1.592120.
Estimated values of coefficients: $A = 0.838441$, $B = 0.095671$, $K = 0.165255$.
Corresponding value of the objective function: 0.034515.

Optimization algorithm: tabu search

Total number of iterations: 1000.
Initial values of coefficients: $A = 0.888234$, $B = 0.092406$, $K = 0.192038$.
Corresponding value of the objective function: 1.289340.
Estimated values of coefficients: $A = 0.836815$, $B = 0.098870$, $K = 0.161006$.
Corresponding value of the objective function: 0.028985.

Optimization algorithm: genetic algorithm

Total number of iterations: 1000.
Initial values of coefficients: $A = 0.904815$, $B = 0.035697$, $K = 0.168398$.
Corresponding value of the objective function: 0.456995.
Estimated values of coefficients: $A = 0.845696$, $B = 0.098815$, $K = 0.158820$.
Corresponding value of the objective function: 0.027871.

2.4. Optimization in estimating coefficients of the operational finite element model

A large variety of optimization algorithms for bound constrained problems were designed and tested for efficiency in searching the objective function minimum with respect to selected coefficients of the operational finite element model. Several functions were analyzed to deal with constraints, and the barrier function was slightly more advantageous than the exterior penalty function. As preliminary investigations showed, only two classes of optimization algorithms were satisfactory with respect to computational performance, due to the large scale of the problem investigated: the variable metric approach (Bazaraa *et al.*, 2006; Jongen *et al.*, 2004; Nash and Sofer, 1996; Zhang *et al.*, 1999) and the trust region method (Bazaraa *et al.*, 2006; Dennis *et al.*, 1997; Gay, 1984; Nocedal and Wright, 2006; Xiaojiao and Shuzi, 2003). Only the two final algorithms were applied to estimate the coefficients. The trust region algorithm was combined with the secant-updating quasi-Newton procedure to approximate the Hessian (the BFGS update), and, in the case of a poor selection of the starting point, the model/trust approach was used to promote convergence.

To exemplify the procedure of estimating the coefficients of the operational finite element model, the transient bound water diffusion in wood was analyzed, and the coefficients required to compute the diffusion coefficient were estimated.

Details of the exemplary instance

Species: Scots pine wood.
Direction: radial.
Number of estimated parameters – 4:

- σ – surface emission coefficient, [m/s]
- D_0 – constant in the empirical model for the diffusion coefficient, [m^2/s]
- a – coefficient in the empirical model for the diffusion coefficient, [–]
- m_e – mass at equilibrium, [kg].

The empirical model for the diffusion coefficient is a part of the operational finite element model of the transient bound water diffusion in wood.

Optimization method: variable metric

Total number of iterations: 59 excluding iterations for computing gradients.
Initial values of coefficients:

$$\begin{aligned}
\sigma &= 5 \cdot 10^{-7}\ \mathrm{m/s} \\
D_0 &= 2.2 \cdot 10^{-10}\ \mathrm{m^2/s} \\
a &= 1.2 \\
m_e &= 20.6\ \mathrm{g}
\end{aligned}$$

Corresponding value of the objective function: 0.0825344.
Estimated values of coefficients:

$$\begin{aligned}
\sigma &= 5 \cdot 10^{-7}\ \mathrm{m/s} \\
D_0 &= 2.2 \cdot 10^{-10}\ \mathrm{m^2/s} \\
a &= 1.2 \\
m_e &= 20.59\ \mathrm{g}
\end{aligned}$$

Corresponding value of the objective function: 0.0730615.

Optimization method: trust regions

Total number of iterations: 29 excluding iterations for computing gradients.
Initial values of coefficients:

$$\begin{aligned}
\sigma &= 5 \cdot 10^{-7}\ \mathrm{m/s} \\
D_0 &= 2.2 \cdot 10^{-10}\ \mathrm{m^2/s} \\
a &= 1.2 \\
m_e &= 20.6\ \mathrm{g}
\end{aligned}$$

Corresponding value of the objective function: 0.0825344.
Estimated values of coefficients:

$$\begin{aligned}
\sigma &= 3.53276 \cdot 10^{-7}\ \mathrm{m/s} \\
D_0 &= 1.56868 \cdot 10^{-10}\ \mathrm{m^2/s} \\
a &= -0.281408 \\
m_e &= 20.4969\ \mathrm{g}
\end{aligned}$$

Corresponding value of the objective function: 0.00157855.

3. Comparison of algorithms and results

Validation of the empirical equations (Section 2.3) and the operational finite element model (Section 2.4) filled with the estimated coefficient values was performed by determining the similarity between experimental data and results predicted by the model: locally – the local relative error and globally over the process duration – the global relative error (Weres and Jayas, 1994; Olek *et al.*, 2003). The global relative error was recognized as the main measure of the coefficient estimation quality by a given optimization algorithm. Other measures were also used to assess the algorithm performance, and the most important were: the minimum value of the objective function and the number of iterations to find the minimum of this function, excluding those for gradient computation.

In the case of the 3-parameter empirical equation for the water transport in corn kernels, the variations in the objective function values with the consecutive iterations were exemplified in Figs. 2-4, respectively for the algorithms of simulated annealing, tabu search and genetic algorithm. Additional information characterizing the optimization procedures was given in Table 1. Short running time of the algorithm corresponded only to proceeding the empirical equation, and not the mathematical structural model of the investigated process.

Table 1. Comparison of optimization algorithms applied to estimate coefficients of 3-parameter empirical equation for water transport in corn kernels

Optimization algorithm	Relative humidity of air [%]	Min. value of the objective function [–]	Global relative error [%]	Algorithm running time [ms]	No. of iterations to find the minimum
Simulated annealing	30	0.039478	3.01	160	389
	40	0.039316	3.01	145	727
	50	0.034515	2.66	184	29
Tabu search	30	0.037516	2.94	598	324
	40	0.036630	2.91	596	358
	50	0.028985	2.43	597	525
Genetic algorithm	30	0.031588	2.70	2591	871
	40	0.036467	2.90	2598	400
	50	0.027871	2.39	2588	812

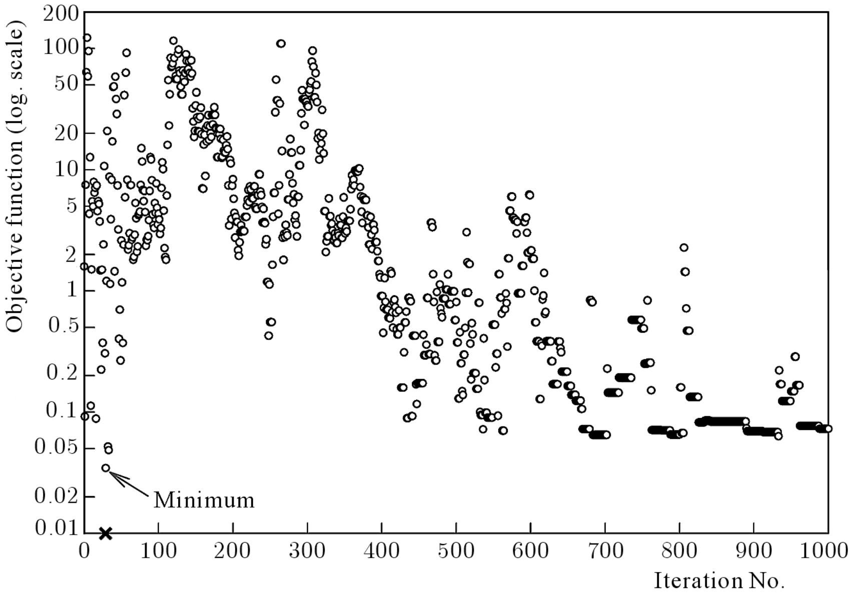

Fig. 2. Objective function vs. iteration number – simulated annealing, 3-parameter empirical equation for water transport in corn kernels, relative humidity 50%

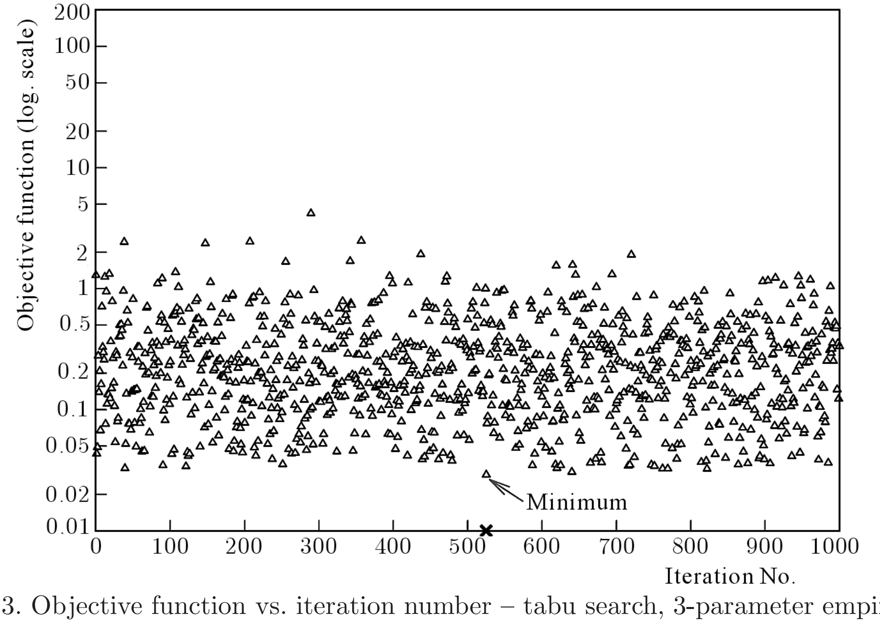

Fig. 3. Objective function vs. iteration number – tabu search, 3-parameter empirical equation for water transport in corn kernels, relative humidity 50%

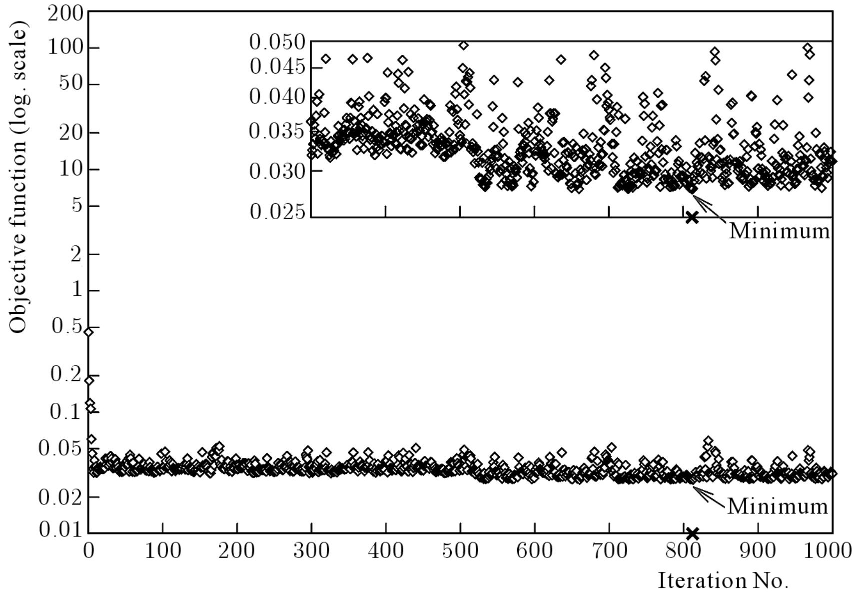

Fig. 4. Objective function vs. iteration number – genetic algorithm, 3-parameter empirical equation for water transport in corn kernels, relative humidity 50%

For the coefficient estimation performed for the operational finite element model corresponding to the transient bound water diffusion in wood, the exemplary values of the objective function varying with iterations were shown in Fig. 5 (the variable metric algorithm) and Fig. 6 (the trust region algorithm). Quality of the coefficient estimation was presented in Fig. 7. Satisfactory results for the trust region algorithm (the global relative error $e_2 = 0.63\%$) were achieved for all the investigated instances, and the variable metric approach was unsuccessful for several of them.

4. Conclusions

The analysis of optimization algorithms implemented to estimate coefficient values of the operational finite element model of heat and mass transport in biomaterials, with the use of the original inverse FEA software developed by the authors, allowed us to compare the algorithms and formulate the following conclusions:

1. All the analyzed optimization algorithms integrated with the inverse FEA software were capable of solving the inverse finite element problems investigated.

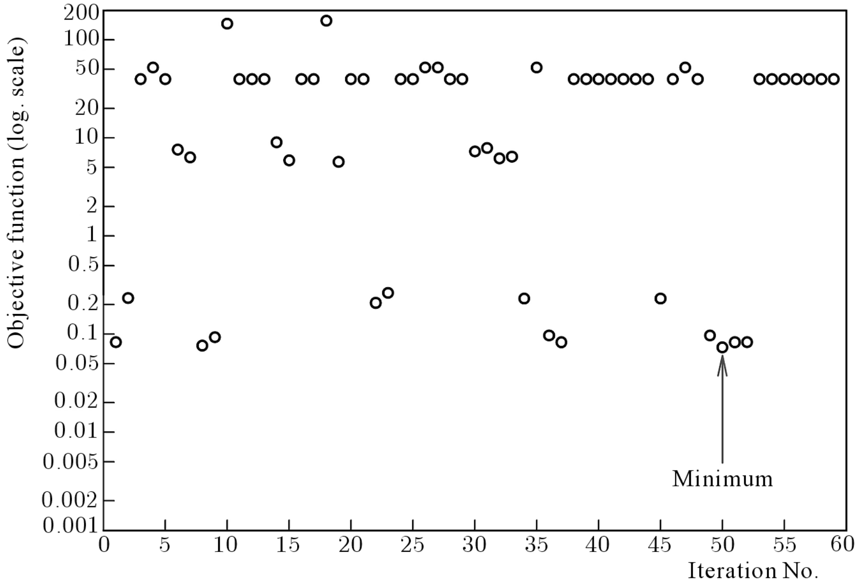

Fig. 5. Objective function vs. iteration number – estimation of four coefficients by the variable metric algorithm, the operational finite element model corresponds to the transient bound water diffusion in Scots pine wood

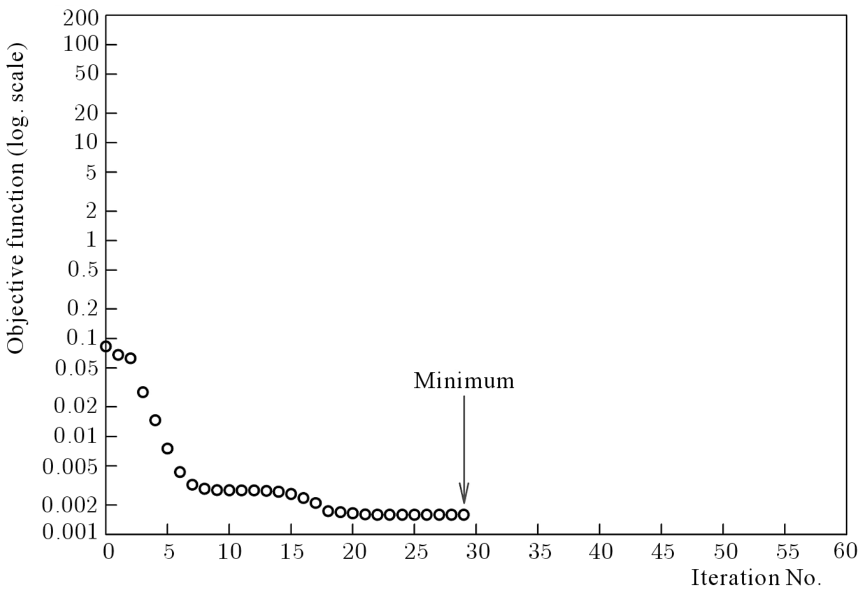

Fig. 6. Objective function vs. iteration number – estimation of four coefficients by the trust region algorithm, the operational finite element model corresponds to the transient bound water diffusion in Scots pine wood

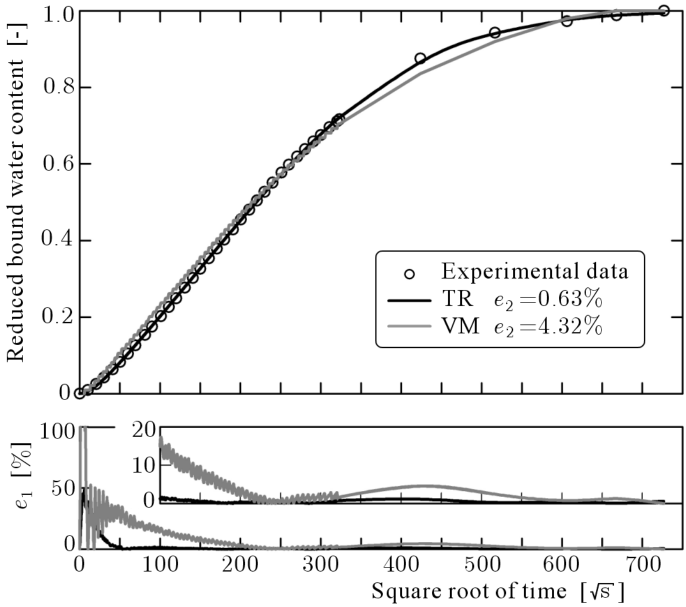

Fig. 7. Similarity between experimental data and results predicted by the operational finite element model with four coefficients estimated by the variable metric (VM) and trust region (TR) algorithms. The relative errors are denoted by e_2 (global) and e_1 (local). The model corresponds to the transient bound water diffusion in Scots pine wood

2. At the stage of optimization in constructing empirical equations, the most precise results were obtained by the genetic algorithm. However, due to computational complexity of this approach, the algorithm running time for the coefficient estimation was definitely the highest. The simulated annealing algorithm was the fastest in terms of the run-time performance, but due to the estimated uncertainty of results it was unsatisfactory. The tabu search algorithm was satisfactory both in the coefficient estimation running time and in precision of the results.

3. At the stage of optimization for estimating the coefficients of the operational finite element model, the best performance for the large scale computation was achieved by the trust region algorithm, and the estimated uncertainty of results in all the instances investigated was the most satisfactory for this algorithm.

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Porównanie algorytmów optymalizacji w analizie odwrotnej transportu ciepła i masy w biomateriałach

Streszczenie

Znaczenie analizy odwrotnej w oszacowywaniu wartości współczynników transportu ciepła i wody w złożonych materiałach pochodzenia biologicznego stale wzrasta. Dzięki zastosowaniu tej metody można zwiększyć dokładność prognozowania procesów transportowych w porównaniu do symulacji opartych na współczynnikach, których wartości są określane wyłącznie metodą eksperymentów naturalnych. Uzyskiwana poprawa dokładności jest niezmiernie przydatna w analizie, projektowaniu i zarządzaniu większością procesów technologicznych w przemyśle rolno-spożywczym i drzewnym. W ostatnich latach zostało opracowanych wiele algorytmów optymalizacji do rozwiązywania zagadnień odwrotnych. W niniejszej pracy poddano analizie i porównano działanie następujących algorytmów: symulowane wyżarzanie, poszukiwanie z tabu, algorytm genetyczny, algorytm zmiennej metryki oraz algorytm obszarów zaufania. Wyniki wskazały, że chociaż wszystkie algorytmy potrafiły oszacować wartości współczynników, pojawiły się różnice w ich działaniu i ze względu na dużą złożoność obliczeniową rozpatrywanego problemu tylko procedura obszarów zaufania przynosiła satysfakcjonujące wyniki.

Manuscript received February 11, 2009; accepted for print April 8, 2009