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Integration of experimental and computational methods for identifying geometric, thermal and diffusive properties of biomaterials**

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A b s t r a c t. Knowledge of physical properties of biomaterials is important in understanding and designing agri-food and wood processing industries. In the study presented in this paper computational methods were developed and combined with experiments to enhance identification of agri-food and forest product properties, and to predict heat and water transport in such products. They were based on the finite element model of heat and water transport and supplemented with experimental data. Algorithms were proposed for image processing, geometry meshing, and inverse/direct finite element modelling. The resulting software system was composed of integrated subsystems for 3D geometry data acquisition and mesh generation, for 3D geometry modelling and visualization, and for inverse/direct problem computations for the heat and water transport processes. Auxiliary packages were developed to assess performance, accuracy and unification of data access. The software was validated by identifying selected properties and using the estimated values to predict the examined processes, and then comparing predictions to experimental data. The geometry, thermal conductivity, specific heat, coefficient of water diffusion, equilibrium water content and convective heat and water transfer coefficients in the boundary layer were analysed. The estimated values, used as an input for simulation of the examined processes, enabled reduction in the uncertainty associated with predictions.

K e y w o r d s: biomaterials, heat and matter transport, 3D geometry meshing, inverse finite element, system integration

INTRODUCTION

Computer predictions of heat and water transport in complex agri-food and forest products are essential for designing and managing advanced technological processes and controlling the quality of products. Uncertainty of such modelling depends on the adequacy and reliability of data used to represent the geometric, thermal and diffusive properties of biomaterials in mathematical structures. In the case of heating, cooling, drying, and rewetting it has generally been accepted that the 3D geometry, thermal conductivity, specific heat, coefficient of water diffusion, equilibrium water content and convective heat and water transfer coefficients in the boundary layer are the most important quantities affecting the accuracy of modelling (Chen *et al.*, 2009; Fanta *et al.*, 2014; Olek *et al.*, 2011; Nowakowski *et al.*, 2013; Perré and Turner, 2007; Weres and Jayas, 1994; Weres and Olek, 2005; Wu *et al.*, 2004). Experimental approaches to determine the physical properties listed above have not been effective. The reason is in the complexity of agri-food, wood and wood-based products, and in the transient, quasi-linear character of the processes.

Insufficient and often erroneous and contradictory knowledge of geometric, thermal and diffusive properties of biomaterials leads to inappropriate control of thermal treatment and storage conditions, with a consequence of deterioration of the quality characteristics of products. Therefore, indirect approaches combining experimental and computational methods have emerged to acquire trustworthy values of the physical properties of biomaterials and to enhance representation of the adequate data in numerical models for predicting the heat and water transport processes. The authors analysed and combined the following groups of methods:

3D geometry modelling of investigated products based on the algorithms of initial processing, edge detection and 3D shape measurement of investigated products (Frączek and Wróbel, 2009; Nowakowski *et al.*, 2013; Rogge *et*

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al., 2014; Szczypiński *et al.*, 2015; Weres *et al.*, 2014a). Problems were found in the studies to attain satisfactory representation of the 3D product geometry, including external surfaces and internal boundaries between components, for further implementation in numerical models of the transport processes. Additionally, 3D geometry modelling can be supported with algorithms of visualization of changes in the properties during heat and water transport processes in space and time (Balcerzak *et al.*, 2015; Fanta *et al.*, 2014; Klaas *et al.*, 2013; Leng *et al.*, 2013; Pieczywek *et al.*, 2011; Weres *et al.*, 2014a; Zhang, 2013). Further improvements in algorithms for fast visual representation of 3D geometry models, enhanced with visualization of changes in physical properties in space and time during thermal and diffusive processes are needed.

Inverse and direct finite element analysis based on the algorithms of identification of thermal and diffusive properties of investigated products and prediction of the product behaviour during heat and water transport processes (Nguyen and Boyce, 2011; Olek *et al.*, 2005, 2011; Ruggiero *et al.*, 2011; Siatkowski *et al.*, 2010a; Weres and Olek, 2005; Weres *et al.,* 2009). Problems of estimation of unknown or unreliable property values were discussed in the papers, and further research is needed to improve the algorithms for reducing the uncertainty of mathematical modelling.

The objective of the study was to integrate experimental and computational methods to design an information system which can enhance the identification of geometric, thermal and diffusive properties of agri-food and forest products subjected to heat and water transport processes during heating, cooling, drying, and rewetting operations. It was assumed that the algorithms being proposed would take into account the transient and quasi-linear character of the heat and water transport, non-homogeneity and anisotropy of the analysed product, irregularity of its 3D geometry, and variation in the microclimate conditions. It was also assumed that all computations would be performed by an information system consisting of integrated components and interfaces, and the results would be validated.

MATERIALS AND METHODS

The following biomaterials were used to provide experimental data for the validation of the software system: maize kernels of the Clarica hybrid variety (FAO 280) produced by Pioneer and grown at the Research and Education Centre of the Poznan University of Life Sciences in Poland, segments of carrot roots (*Daucus carota* L.), Scots pine (*Pinus sylvestris* L.) and European beech (*Fagus sylvatica* L.), and commercial and laboratory-made wood-based panels *ie* particleboard, medium density fibreboard (MDF) and oriented strand board (OSB). The examined biomaterials were characterized by non-homogeneity and anisotropy, and irregular geometry. The following properties were selected for the process of identification: 3D nodal coordinates of the finite element mesh of a product, thermal conductivity, coefficient of water diffusion and convective water transfer coefficient in the boundary layer. Material samples were prepared according to Czajkowski *et al.* (2016), Olek *et al.* (2005), and Siatkowski *et al.* (2010b).

The approach was based on combining experimental results and algorithms appropriate for image processing, edge detection, 3D geometry modelling, and inverse and direct finite element analysis. The algorithms, referenced in section Introduction and described in the following paragraphs, were integrated and coded within an original software system called BioProcessSoft with the aim to improve the accuracy and performance of identification of geometric, thermal and diffusive properties of biomaterials.

Product samples were individually embedded in a synthetic resin block, and then two small holes were drilled in the opposite corners of the resin block to automate further processing of consecutive cross-section images. At the image acquisition stand each sample was cut by a microtome into layers of a selected thickness, and for each layer a macro photograph was taken (Nikon D7000, AF-S VR Micro-Nikkor 105 mm f/2.8G IF-ED). The first image was initially processed to facilitate the analysis, and all the consecutive images were automatically corrected. Product external boundaries and boundaries between internal components were detected by the improved Canny algorithm. The size of a structural finite element mesh was input to the system appropriately for a product, and the 3D mesh of isoparametric finite elements was automatically generated for all the layers as the output. Global coordinates of the mesh nodes were automatically measured in pixels, converted into length unit in the metric system, and saved in a form acceptable for other modules of the software. The improved algorithms were integrated to improve the performance and accuracy of edge detection operators and finite element mesh generation.

Three-dimensional visualization of products extended by visualization of changes in their properties in space and time was based on concepts described by Weres *et al.* (2014a). The visualization software was enhanced and integrated within the system as the BioVis subsystem. The geometry of an investigated product was represented by 3D, curvilinear, isoparametric finite elements built over the nodal coordinates determined in the 3DMeshNode subsystem. A wire-frame, solid and textured model approaches were chosen to visualize the product geometry, and they were supplemented with the NURBS smoothing, illumination and reflection enhancements. Affine transformation methods were implemented to perform translation, rotation and scaling. A possibility of layer cropping along any of the three coordinate system axes was proposed to remove portions of a product and expose its interior. Differentiation in a selected quantity in space is represented by colours smoothly varying between the nodes and related to the colour scale bar. A complementary approach based on the parametric 3D modelling in the 3ds Max environment described in Balcerzak *et al.* (2015) was also used to construct 3D geometry models.

A methodological approach to inverse problems of identifying thermal and diffusive properties important for the heat and water transport was outlined by Weres and Olek (2005), Weres *et al.* (2009, 2014b). The mathematical model describing the structure of the heat and mass transport processes in biomaterials was represented as a system of quasi-linear differential equations of heat conduction and water transfer with the initial and boundary conditions of the first or third kind, as required in a given analysis. Experimental data were acquired for several empirical systems at different stands. To acquire data in the case of transient heat transfer an experimental setup was constructed according to the guidelines of Czajkowski *et al.* (2016). The setup was equipped with thermocouples for temperature measurements in established locations inside a product, at its surface, and at the outer layer, and at specified time instants. The thermocouples were connected to automatic data logging systems. The results of experiments for transient heat transfer were used as necessary and sufficient input data for the identification of thermal conductivity.

In the case of water sorption and desorption another setup was built to obtain data (Olek *et al.*, 2005, 2011; Olek and Weres, 2007). In this setup, air of controlled temperature and relative humidity flows around a sample of a product of known and uniform initial moisture content. Due to the unique design of the apparatus, it is possible to control precisely the temperature (inaccuracy ±0.1°C) and the relative humidity of air (inaccuracy ±0.5%). Consequently, long-lasting experiments, even over 4 weeks, could be conducted. Two laboratory balances were employed in the apparatus to register automatically changes in sample mass at selected time instants. The apparatus was additionally equipped with a unique system for automatic taring of the unloaded balances during experiments, which improved the stability of balance operation in long-lasting experiments. A computer system controlling the apparatus enabled registering changes in mass during experiments and registering parameters of flowing air. The results were used as input data for the identification of the coefficient of water diffusion, convective water transfer coefficient in the boundary layer and equilibrium water content. In the inverse identification procedure the experimental values of the moisture content were compared to predicted moisture content values at corresponding time instants, averaged over the domain of a sample.

The authors algorithms and software (Weres and Olek, 2005; Weres *et al.*, 2009, 2014b) were put forward and integrated in this work, and used for inverse and direct finite element modelling. The finite element algorithms were based on 3D isoparametric curvilinear spatial elements, absolutely stable two- and three-point recurrence schemes of approximation in time, and iterative procedures to deal with equation quasi-linearity. Updated and more effective algorithms for local optimization with constraints (trust region and variable metric methods), and for global optimization (randomization, tabu search, simulated annealing and genetic algorithms), and also hybrid procedures (global optimization algorithms combined with the trust region local approach) were used to minimize the objective functions in the L2-norm, as differences between experimentally measured values of temperature and moisture content and corresponding values predicted in simulation.

The integrated software system and its subsystems were logically verified and empirically validated against functional requirements. Values of the local and global relative errors were computed according to the formulae given by Olek *et al.* (2003) for heat transport problems and Olek *et al.* (2005) for water diffusion problems. The errors were based on comparing the results of computer predictions for heat and water transport in investigated products with the results of laboratory experiments. Values of the product properties identified with the lowest global relative error were taken as inputs to the computer simulation of the examined processes.

The software system called BioProcessSoft was designed in this work as an integration of algorithms developed by the authors for image processing and analysis (subsystem 3DMeshNode), 3D geometry modelling of investigated products (subsystem BioVis), and inverse and direct finite element analysis (subsystem IPS). The overall purpose of the system was to identify, analyze and visualize the geometric, thermal and diffusive properties of agri-food and forest products, and to predict the heat and water transport processes. Additional common components like graphical user interfaces, database and help were also designed within this work, and integrated. The system was developed according to software engineering standards, including quality standards (Gomaa, 2011). The problem domain was analysed and documented in the UML 2.4.1 notation in the Visual Paradigm 11.2 diagramming tool (Visual Paradigm International, Hong Kong), and integration issues were considered on the level of the problem domain analysis by integrating classes and components with their interfaces. The Visual Studio 2013 programming environment (Microsoft Corp., Redmond, WA, USA) with the C# 5.0 and C++/CLI languages was used to develop the software at assumed level of accuracy and performance. The Intel Visual Fortran Composer XE for Windows with the IMSL mathematical libraries (Intel Corp., Santa Clara, CA, USA) was used to code the finite element algorithms and, as the Intel environment was entirely embedded in the Visual Studio 2013, the cross-language component integration was smooth. In the case of geometry modelling and visualization of product properties, the graphical library OpenGL (Free Software License, Silicon Graphics International Corp., Milpitas, CA, USA) was implemented and accessed for the .NET Framework in the C# language with the use of the Tao.OpenGl (the Tao Classic, formerly the Tao Framework, the MIT open source license) and OpenTK (the Open Toolkit Library, the MIT open source license). Particular attention was paid to methods of unifying the data exchange between the subsystems, and to methods of developing integrated user interfaces in the Windows Presentation Foundation (WPF) technology in C# 5.0 available in the Visual Studio 2013.

RESULTS AND DISCUSSION

The integrated software system was developed following the methods described in the section Materials and Methods. After specifying multi-purpose requirements, analysing and diagramming the problem domain and designing the subsystems, the user interfaces were implemented at the top level and operational functions and components were coded at the bottom level. Subsequently, the unit tests were performed and the system was integrated, verified and validated. The startup interface of the BioProcessSoft software system (Fig. 1) enables access to the subsystem interfaces (3DMeshNode, IPS and BioVis).

The heat conduction and water diffusion processes were analysed in biomaterials listed in the section Materials and Methods. Data were processed following the scheme shown in Fig. 2.

Product samples were cut and photographed. Images of product layers were processed, boundaries were detected, isoparametric finite element meshes were generated for the layers and automatically assembled into a single 3D mesh, and the nodal coordinates were saved as the output of the 3DMeshNode. Experiments were performed and data on temperature in selected locations and time instants, and mass changes in time for selected products were collected according to the experimental procedures described in the section Materials and Methods.

The novel version of the IPS subsystem is an inverse problem solver combining the authors finite element algorithms for solving direct parabolic problems of heat conduction and matter diffusion (Weres and Olek, 2005; Weres *et al.*, 2009) with algorithms for solving local and global optimization problems with constraints (Weres *et al.*, 2009). The subsystem is suitable for analysing complex, transient, three-dimensional, quasi-linear, inverse and direct problems of heat and matter transport in non-homogeneous and anisotropic biological materials of irregular shape and with initial and boundary conditions of the first, second and third kind at different parts of the product surface. Identification procedures were used to estimate the thermal conductivity for the heat conduction problems and – in the case of the water diffusion problems – the coefficient of water diffusion and the convective water transfer coefficient in the boundary layer.

The constraint optimization algorithms available in the IPS subsystem (trust region, variable metric, tabu search, simulated annealing, genetic algorithm, and hybrid algorithms) were analysed for each inverse problem under analysis, and the most suited algorithm was selected to minimize the objective function (Figs 3, 4). The estimated property values were used to simulate the examined processes. The uncertainty of modelling emerges from the quality of representing geometry and coefficients in the mathematical model, and it was assessed by computing the global and local relative error values.

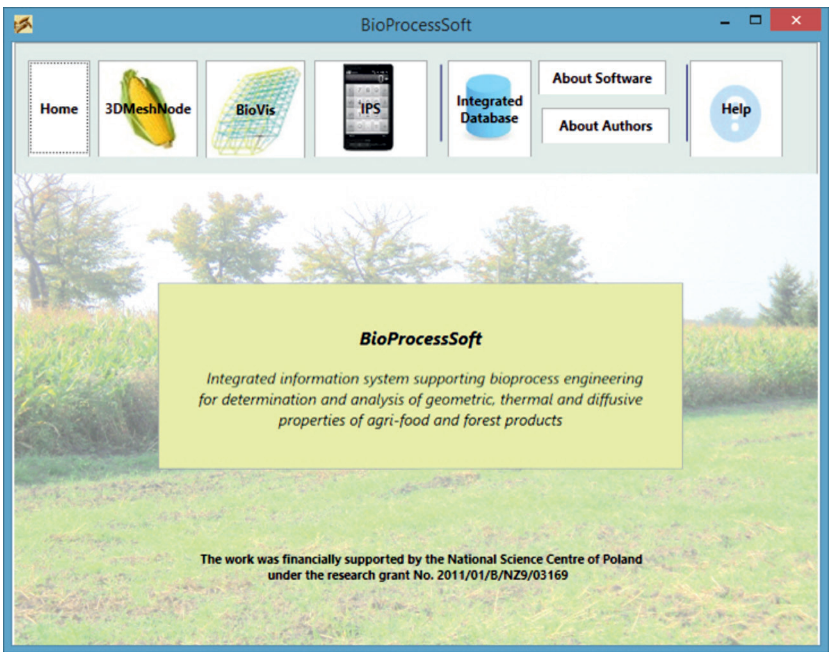

Fig. 1. Startup interface of the BioProcessSoft software system.

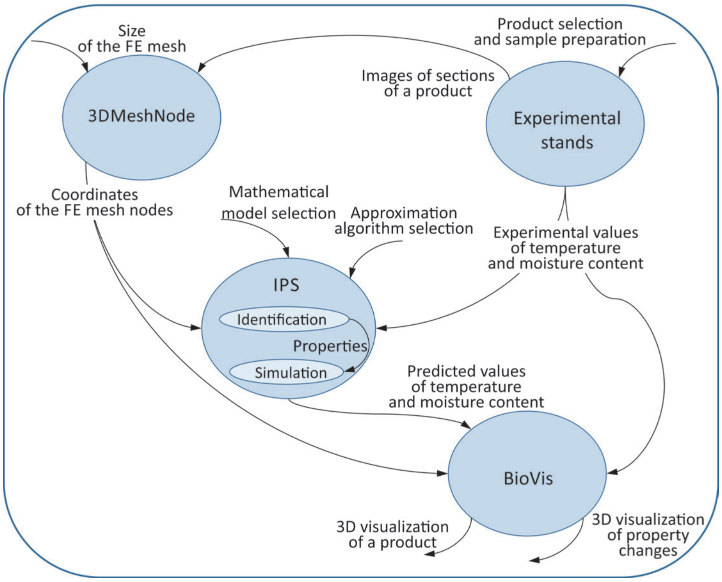

Fig. 2. Scheme of the data input and output for the BioProcessSoft software system.

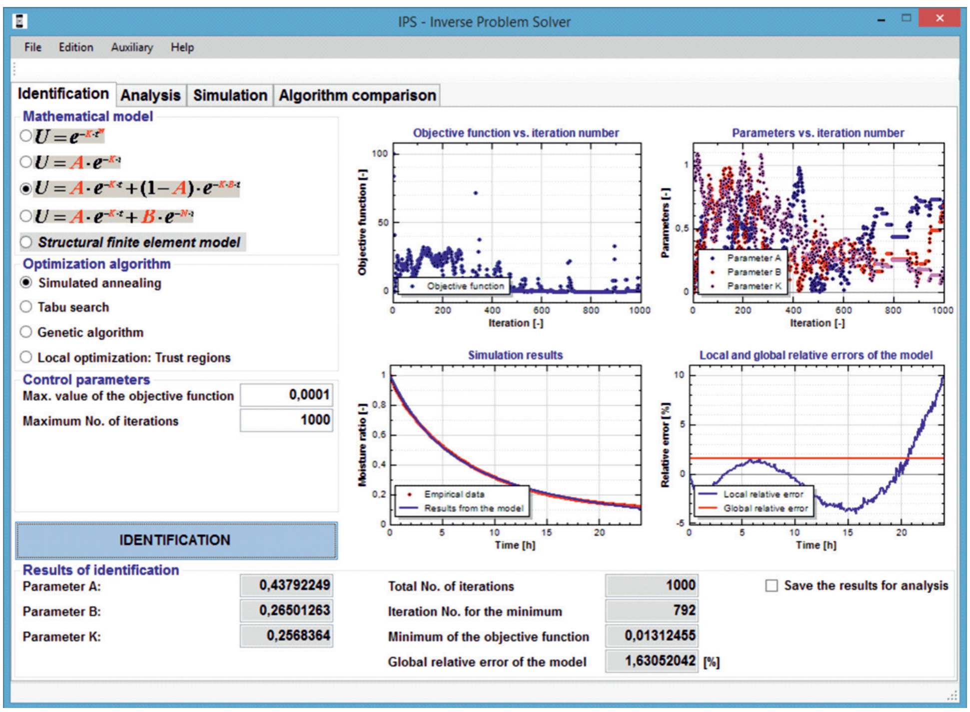

Fig. 3. Selection of a mathematical model and an optimization algorithm, input of control parameters and identification results for the non-structural model and simulated annealing in the IPS subsystem.

The identified geometry data and predicted process performance were used in the BioVis subsystem to visualize the examined products and to visualize changes in product properties. The selected quantity, characteristic for the heat and water transport and resulting from the computer predictions, can be presented as a function of time either in the form of a curve for a selected node or in the form of an animation for the whole product or for a selected portion. It enables a deeper insight into the structure and shows changes in a selected property inside an investigated product. In the models of a maize kernel and a carrot root segment (Fig. 5) the following options were enabled: the NURBS smoothing, illumination, reflection, translation, scaling and layer cropping. A process quantity – the moisture content in a selected node of the kernel – is also presented as a function of time.

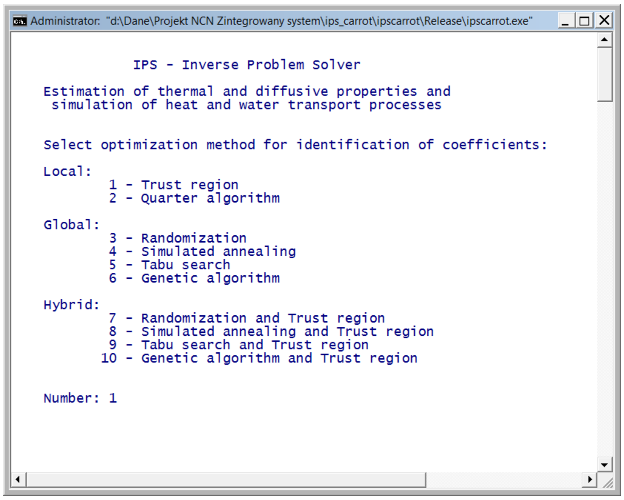

Fig. 4. Menu for optimization methods in the IPS subsystem after selecting identification of coefficients of the structural finite element model as the mathematical model.

A complementary approach was implemented to construct models of the agri-food products on the basis of parametric modelling in the 3ds Max (Fig. 6), with the use of geometry data acquired in experiments and in the 3DMeshNode subsystem.

A reduction in the uncertainty of modelling of heat conduction and water diffusion in the investigated biomaterials was achieved, measured by the values of the global and relative errors of predictions. Both the efficiency and the performance of the software were assessed at subsystem and system levels, design modifications were incorporated into the prototypes until the requirements were met, and finally the geometry and the thermal and diffusive properties of selected products were identified with the use of the novel software system termed BioProcessSoft. Exemplary results are given below.

In the case of identification of the temperature-dependent thermal conductivity in the three anatomic directions of European beech (*Fagus sylvatica* L.) and Scots pine

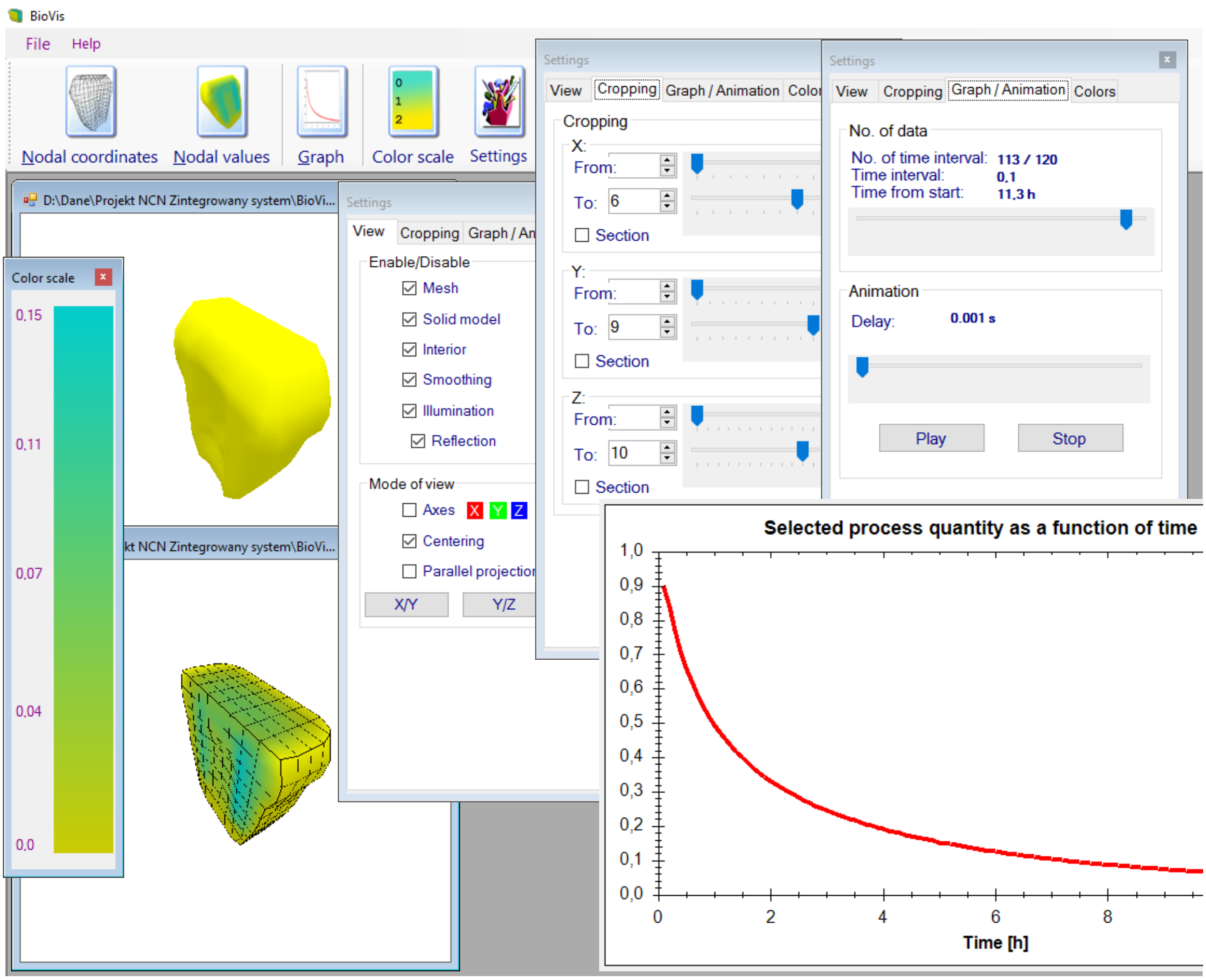

Fig. 5. Visualization of models of a corn kernel and a carrot root segment, and moisture content changes in the kernel prepared in the BioVis subsystem. The FE mesh loaded from the 3DMeshNode and the process quantities loaded from the IPS.

Fig. 6. Visualization of models of a parsley root segment, oat, wheat and corn kernels developed by the parametric modeling (Balcerzak *et al*., 2015) in the 3ds Max.

(*Pinus sylvestris* L.) the global relative error of prediction was reduced to the range of 1-2%, which was a significant improvement in modelling the heat conduction in wood in relation to results reported in the literature (Olek *et al.*, 2003). The results were obtained for the model in which thermal properties were related to temperature and moisture content. When this dependency was neglected and constant values of thermal properties were used, the global relative error reached 20%.

For investigating heat conduction in wood-based panels (particleboard, MDF and OSB), the specific heat was measured in a water calorimeter originally developed to reduce the uncertainty, and the thermal conductivity was identified. The global relative error values for predicting the temperature were in the range from 0.5 to 0.9%. For predictions based on data found in the literature the error ranged from 11.5 to 25.0% (Czajkowski *et al.*, 2016).

In the analysis of the transient bound water transport (processes of adsorption and desorption) in Scots pine (*Pinus sylvestris* L.) and European beech (*Fagus sylvatica* L.), the identification was performed for the two coefficients expressing the dependency of water diffusion on bound water content, and for the three coefficients expressing the expanded convective boundary condition in terms of the equilibrium water content dependent on time. The coefficient of water diffusion was identified for the radial and tangential directions. The global relative error of predictions was in the range from 0.63 to 2.15%, and in the case of neglecting the dependency of the coefficient of bound water diffusion on the water content, the respective error values were up to 5.3%. In the case of traditional methods for determination of the coefficient of water diffusion for wood, based on the boundary condition of the first kind, the local relative error values were reaching 60%. In the case of traditional methods based on the convective boundary condition, the global relative error values approached 20% (Olek and Weres, 2007; Olek *et al.*, 2011).

In the case of water diffusion processes in dried maize kernels, the experimental data on moisture content changes in time were generalized with a three-parameter empirical formula as an input to the procedure of identifying the coefficients of the structural finite element model. Empirical, non-structural models are implemented in the IPS subsystem, as well as the metaheuristic global optimization algorithms, and they were used to estimate the coefficients of the empirical formula. The lowest uncertainty was for the genetic algorithm, but due to computational complexity its performance was unacceptable. The simulated annealing was the best in terms of the runtime performance, but due to the uncertainty of results it was unsatisfactory. The tabu search was used as a compromise between the coefficient estimation running time and the uncertainty of the results – the global relative error was in the range from 1.15 to 1.34%. For large-scale computation in identifying coefficients of the structural finite element model the trust region algorithm was the most satisfactory with respect both to the performance and to the uncertainty of results for all investigated instances. Similar uncertainty was achieved in the case of the global optimization metaheuristics and the hybrid algorithms, but their runtime performance was distinctly worse. The global relative error for the predicted moisture content was in the range from 5.32 to 6.82%, and in the case of taking the coefficient values from the literature it was between 21.46 and 32.72%.

CONCLUSIONS

1. An integrated software system was developed to enhance the identification and analysis of the geometric, thermal and diffusive properties of agri-food and forest products, and to predict the heat and water transport processes during heating, cooling, drying, and rewetting operations, and during storage of the products. Original enhanced algorithms for image analysis, finite element inverse and direct modelling, and for modelling and visualising product geometry and changes in the properties were used.

2. The system components were verified and validated in relation to experimental results for various biomaterials. The functional requirements were met, and the functionality, usability, effectiveness and efficiency were acceptable.

3. An improvement was achieved in computational accuracy and performance, and a reduction of uncertainty of predictions was attained due to estimation of more reliable data on product properties. The software system offers essential support in investigating heat and water transport in agri-food and forest products.

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