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Inverse estimation of model parameters for newborn brain cooling process simulations

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In this work, a three-dimensional simplified computational model was built to simulate the passive thermo-physiological response of part of a newborn's head for neonate's selective brain cooling. Both metabolic heat generation and blood perfusion were considered. The set of model parameters was selected and a sensitivity study was carried out. Analysis of dimensionless sensitivity coefficients showed that the most important are: the contact thermal resistance between the cool-cap and skin, the thermal resistance of the plastic wall material, and deep (arterial) blood temperature. The function specification method was applied to estimate the value of the contact resistance. Two, four and six computationally simulated measurements with different uncertainties were used to adjust random contact resistance value to the assumed one. Results showed that when using only two measurements having 2% of the uncertainty, the error of estimation does not exceed 9.8%. However, when using six measurements having 1% of uncertainty, the resulting estimation is burdened with an error of 0.3% only.

Keywords: inverse method, function specification method, bioheat, brain cooling.

1. Introduction

Perinatal hypoxia and asphyxiation lead to a number of abnormalities of the central nervous system called hypoxic-ischemic encephalopathy (HIE). HIE is the main cause of natal death and disability worldwide.

In recent years, besides the supportive and symptomatic treatment, several therapies have been examined. Hypothermal therapy is one of the therapies commercially used, and it is the most effective and widely considered to be standard care [1].

Lowering the level of brain cell metabolism, reducing cytotoxin generation, and apoptosis prevention can be achieved by reducing brain temperature [2]. During therapy, the neonate's head selectively or the whole body is being cooled to the targeted body temperature, respectively: 34.5° and 33.5° [3]. Hypothermal therapy must be applied as soon as possible, within 6 hours after birth and maintained for 72 h [1, 3]. Statistical research shows [4] that such a therapy is beneficial in term and late preterm newborns with mild and severe hypoxic-ischaemic encephalopathy.

However, still not all of the patients are protected from death or severe disabilities. Therefore, further research needs to be done to develop the technique and increase the efficiency of the method. For example, the following aspects should be explored [2, 4]:

- appropriate cooling methods,
- optimal time window,
- duration of cooling,
- the methodology of controlled rewarming.

Therapies based on hyperthermia or hypothermia influence the homeostasis, causing the biological response of the organism. The body activates thermoregulation mechanisms in order to maintain a favourable temperature. Brain cooling has to be performed in a way that enables controlling brain temperature despite the changes of metabolic heat generation and perfusion rate with respect to the tissue temperature.

Body temperature is being monitored continuously during therapeutic hypothermia and the rewarming phase. Rewarming must be conducted slowly to maintain a gradual temperature increase of 0.5° per hour [5] as rapid changes in cerebral blood flow may cause hemorrhage [3]. Thus, a crucial parameter in the case of the therapy is the brain temperature, which cannot be measured directly but can be estimated using computational modelling, including bioheat transfer processes and environmental impact.

Thermophysiological models have been a focus of the number of research over decades. The first mathematical descriptions of the human body interaction with the environment have been proposed at the turn of the 19th and 20th centuries. More recent models mostly concern human body thermophysiological responses when exposed to different environmental conditions, e.g., [6–9]. That allow the mathematical description of thermoregulation reactions, modelling heat balance for isolated body parts, and further evaluation of thermal comfort and sensation. The extensive review of thermophysiological models and their applications, as well as their detailed classification, were performed by Katić *et al.* [9].

Thermophysiological models include two systems: passive (controlled) and active (controlling). The passive system concerns heat transfer phenomena within human tissues, internal heat sources (metabolism and blood perfusion), and heat exchange between the human body and environment. The active system is responsible for maintaining the core temperature in changing ambient conditions through vasoconstriction, vasodilation, shivering and sweating [9].

Parameters of human tissues and the environmental conditions serve as the passive model inputs. The purpose of the present work is to test model sensitivity on the chosen inputs to distinguish the most important ones. The second aim is to examine the method of establishing the unknown model parameter, which is the contact thermal resistance between the cooling devices and the skin surface. The model must be certainly validated based on the real therapy data. The experimental and numerical studies are briefly discussed in the next sections. Furthermore, the sensitivity analysis, as well as an implementation of the function specification method [10, 11] used for inverse estimation of contact thermal resistance, are briefly described below.

2. Experiments

During the therapy, the neonate is placed in the opened incubator provided with devices monitoring vital signs, heated mattress and the radiant warmer placed over the patient (Fig. 1).

Selective brain cooling is performed using the Olympic Cool-Cap System [12] (shown schematically in Fig. 2) and lasts for about 72 h. The infant's head is cooled using the cool-cap in which water flows (Fig. 3) and on the top of which, the cool-cap retainer and insulating outer cap are applied [12]. The average cooling water temperature is maintained by a cooling unit. Head, during the cooling phase of the therapy, is protected from being irradiated by the thermal screen (Fig. 1).

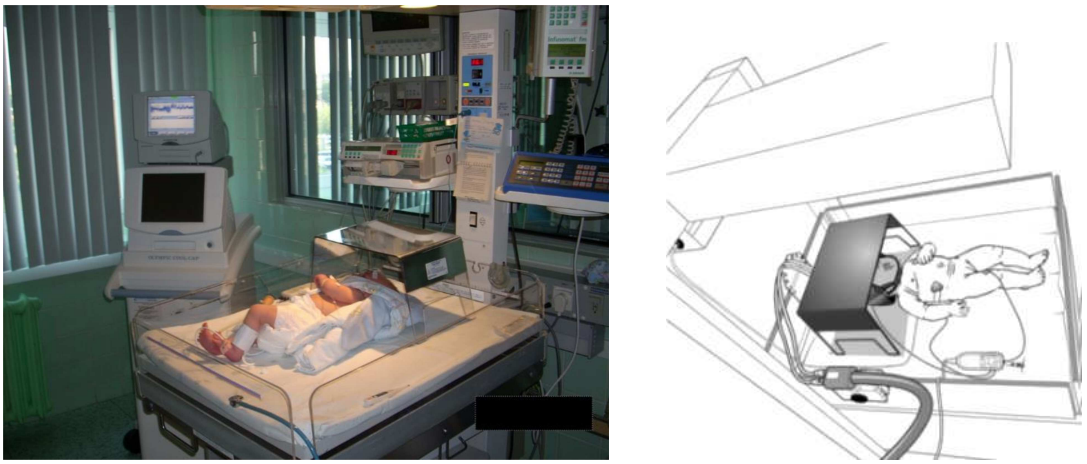

Fig. 1. Patient in the incubator. Courtesy of the Univ. Clinical and Olympic Cool-Cap. Used by permission.

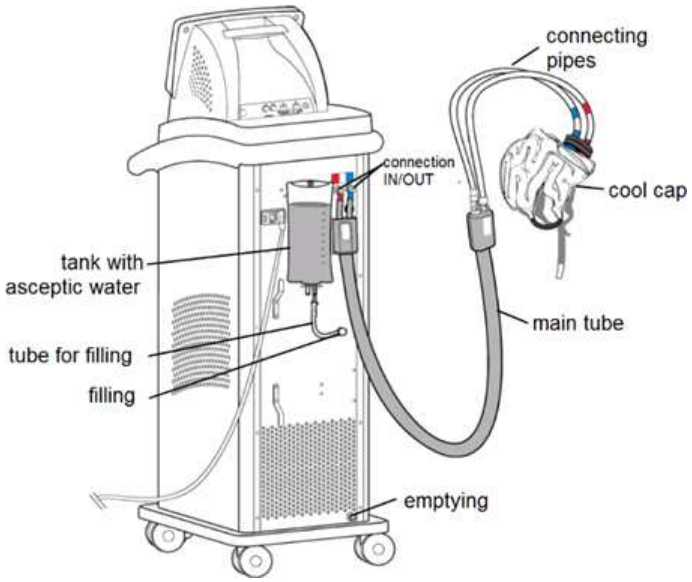

Fig. 2. Accessories of Olympic Cool-Cap System. Courtesy of Olympic Cool-Cap. Used by permission of the Polish representative office.

Fig. 3. Application of cool-cap. Courtesy of Olympic Cool-Cap. Used by permission of the Polish representative office.

Measurements are carried out at the University Clinical Hospital in Opole using specially designed and manufactured devices capable of determining the histories of heat rate retrieved by the cooling medium (water) during therapy [13]. It is done by flow rate and water temperature

measurements (Figs 4–6). Moreover, the temperature of the skin over the liver, forehead temperature, as well as rectal temperature, are simultaneously recorded by the cooling device [12, 13]. In addition, the temperature and relative humidity of the ambient air, as well as the actual radiant temperature, is recorded.

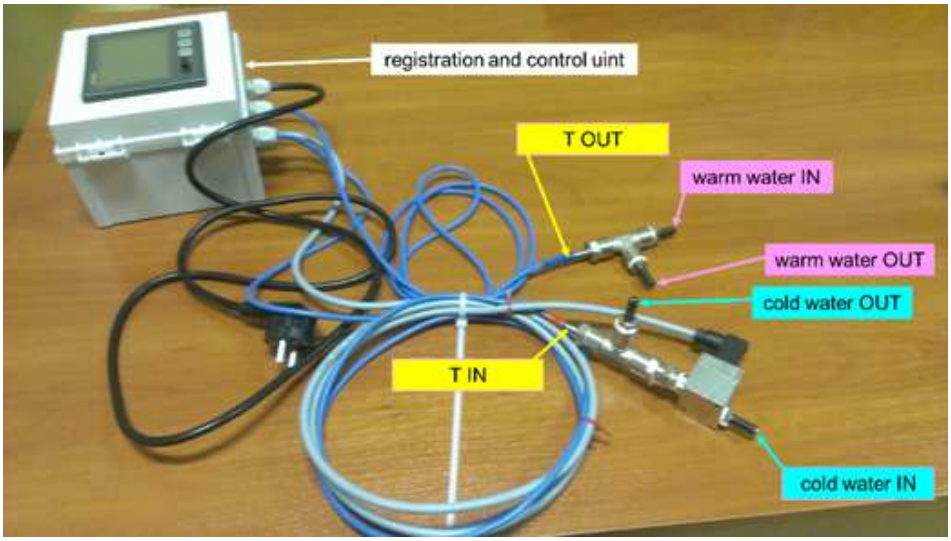

Fig. 4. Experimental setup.

Fig. 5. Experimental setup connected with the cooling device.

Fig. 6. Close-up on the connection.

3. Numerical direct model

A simplified numerical model of the heat transfer that occurs during therapy is built. The model, built by means of ANSYS® Fluent, Release 17.2 code [14], includes the water flowing inside the plastic channels being in contact with the tissues: an outer skin, inner skin, fat, bone, and brain. The water channel is surrounded by an air zone as it is presented in Figs 7 and 8.

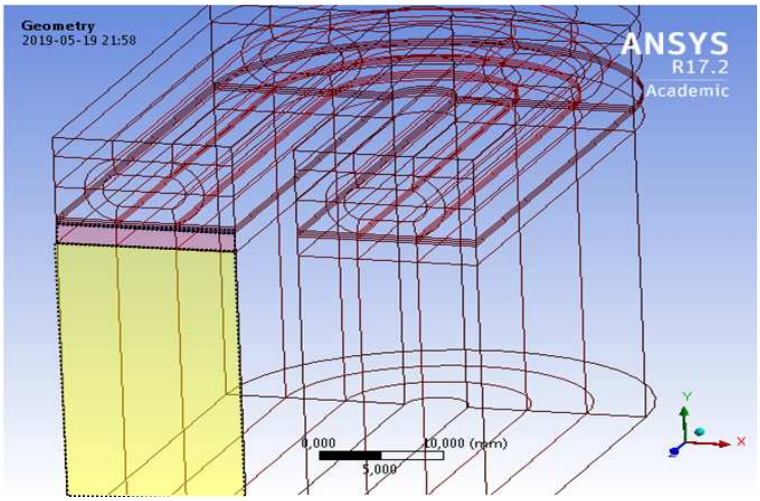

Fig. 7. 3D model geometry. Images used by courtesy of ANSYS, Inc.

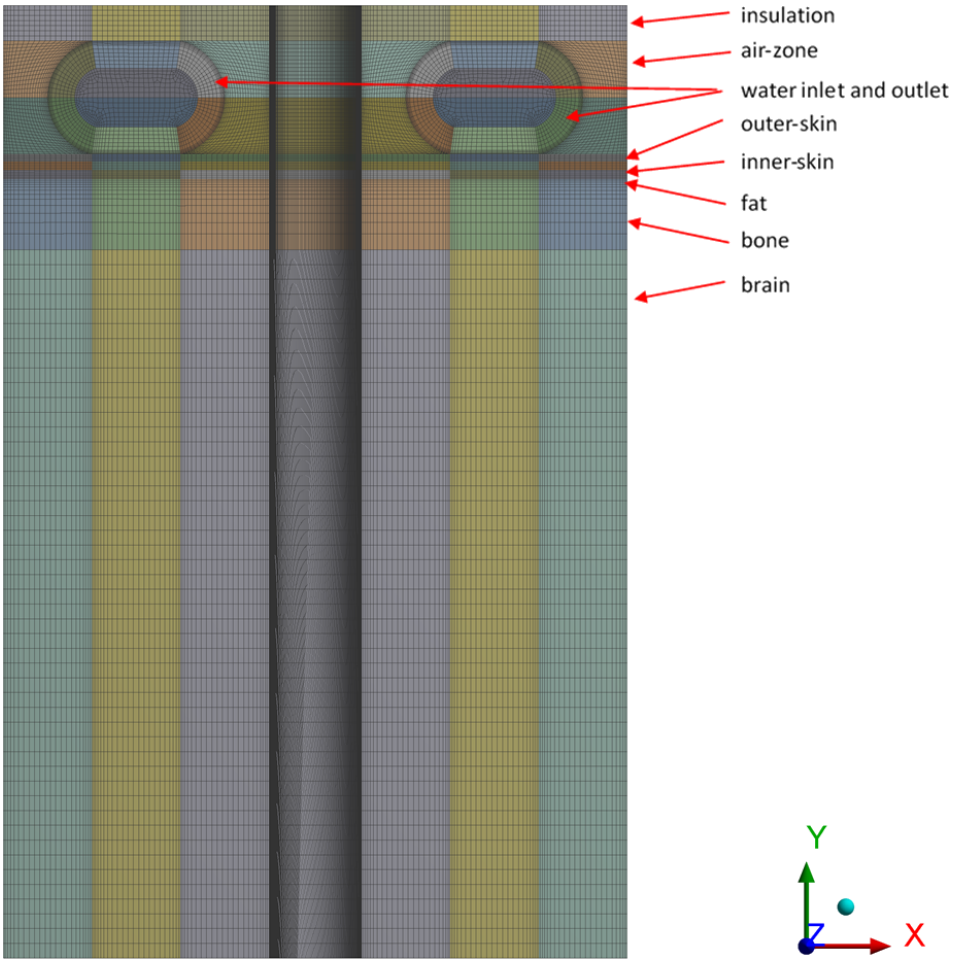

Fig. 8. Cross-section of the computational domain. Images used by courtesy of ANSYS, Inc.

For turbulent heat transport in the water channel, the energy equation is being solved by ANSYS Fluent [14]:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) = \frac{\partial}{\partial x_j}\left(k_{eff}\frac{\partial T}{\partial x_j} - u_i\tau_{ij}\right) + S_h, \tag{1}$$

where t stands for time, ρ – density, E – total energy (enthalpy), u – velocity, p– pressure, k_{eff} – effective conductivity that includes turbulent thermal conductivity, T – temperature, τ – deviatoric stress tensor, and S_h is an internal heat source.

Effective conductivity is described as follows:

$$k_{eff} = k + \frac{c_p\mu}{\mathrm{Pr}}, \tag{2}$$

where c_p is a specific heat capacity, μ is the viscosity of the fluid, and Pr is a Prandtl number [14].

Deviatoric stress tension (τ) in the described model is neglected as a representative of viscous heating [14]. Moreover, there are no internal sources in the water flowing in the pipe, thus $S_h = 0$. As the analysis presented in this article is based on the steady-state calculations, it does not contain the time-dependent term.

The following energy equation is used for modelling steady-state heat transfer in the tissues [8, 15, 16]:

$$\nabla(k\nabla T) + \rho_b c_b \omega_t (T_a - T_t) + \dot{q}_{met,t} = 0, \tag{3}$$

where subscript b refers to 'blood', t refers to 'tissue', and a means arterial. The basic thermoregulation models are implemented by two volumetric sources that are related to ω_t – blood perfusion and $\dot{q}_{met,t}$ – metabolic heat generation rate, given by:

$$\dot{q}_{met,t} = \dot{q}_{met,t,0}\left(Q_{10}^{(T_t - T_0)/10}\right), \tag{4}$$

where $\dot{q}_{met,t,0}$ refers to the metabolic heat generation rate in temperature T_0, and the Q_{10} factor describes changes in chemical reaction velocity due to temperature changes. Its value is usually assumed to be 2 [8, 17, 18].

The increase of perfusion rate depends linearly on the variations of metabolic heat generation, what is here described using the blood perfusion energy equivalent term called as β W/(m^3 K) [19]:

$$\beta = \rho_b c_b \omega_t, \tag{5}$$

$$\Delta\beta = \mu\Delta\dot{q}_{met}. \tag{6}$$

The proportionality coefficient μ is estimated empirically and it takes value $\mu = 0.932$ 1/K [20]. The metabolic source terms of the bioheat Pennes equation (for inner skin, fat, and brain) have been implemented in ANSYS Fluent numerical model using user defined function (UDF).

The additional contact thermal resistance between the cooling channel and the skin was taken into consideration. The material properties (both living tissues and passive materials), as well as initial metabolic heat sources and perfusion rates, have been also assumed based on the literature sources and are summarized in Table 1.

The ambient temperature and heat transfer coefficient, as well as water flow speed, were estimated based on the experimental data (Table 2).

The preliminary model aims to verify adopted assumptions. The total heat transfer rate that is transferred into cooling water is computed using the above described model. The sensitivity of the simulated total heat transfer rate on selected model parameters is presented in the next section.

Table 1. Thermal parameters of tissues and materials used in the model.

Tissue/material	Thermal conductivity k [W/mK]	Heat capacity c [J/kgK]	Density ρ [kg/m^3]	Perfusion rate ω [s^{-1}]	Metabolic heat generation rate q_m [W/m^3]
Outer skin	0.4700	3680	1085.000	0.0000000	0.0
Inner skin	0.4700	3680	1085.000	0.0011000	631.0
Fat	0.1600	2300	850.000	0.0000036	58.0
Bone	0.7500	1700	1357.000	0.0000000	0.0
Brain	0.5000	3805	1000.000	0.0170000	6454.4
Water	0.6000	4182	998.200	–	–
Air	0.0242	1006	1.225	–	–
Cool-cap wall	0.1500	2310	700.000	–	–
Insulation	0.0500	2310	700.000	–	–

Table 2. Measured parameters of the model.

Parameter	Unit	Value
Ambient temperature	T_{amb} [K]	296.0
Convective heat transfer coefficient	h [W/m^{2}K]	4.000
Water flow velocity	u [m/s]	0.209

4. Sensitivity analysis

Sensitivity analysis can serve as a tool in the identification of the key parameters that influence the results of numerical simulation models or measurements. Both are affected by errors, whether related to undertaken assumptions or measurement uncertainty.

The following parameters were considered in terms of sensitivity analysis of the described model: contact thermal resistance between the cool-cap and skin, thermal resistance of the plastic wall material, deep (arterial) blood temperature, water velocity in cool-cap channels, heat transfer coefficient between the cooling cap and the environment, ambient temperature.

The first step of the analysis was to compare them all to each other to identify the most important ones. For this purpose, for each model parameter Y (at point Y^*), the *dimensionless sensitivity coefficient* has been defined [11]:

$$Z_d = \frac{\partial \dot{Q}}{\partial Y} \frac{Y^*_{\max} - Y^*_{\min}}{\dot{Q}_{\max} - \dot{Q}_{\min}} \approx \frac{\dfrac{\dot{Q}\left(Y^* + \delta_Y Y^*\right) - \dot{Q}\left(Y^* - \delta_Y Y^*\right)}{\dot{Q}_{\max} - \dot{Q}_{\min}}}{\dfrac{\left(Y^* + \delta_Y Y^*\right) - \left(Y^* - \delta_Y Y^*\right)}{Y^*_{\max} - Y^*_{\min}}}, \tag{7}$$

where Z_d is a dimensionless coefficient, $\dot{Q}$ – measured heat flux rate being transferred from the head to the water in steady-state conditions, Y^* – parameter being estimated, subscripts '*max*' and '*min*' refer to the maximum and minimum values of the given model parameter in the carried out sensitivity analysis, δ_Y – coefficient (greater than 0) accounting for deviation of the model parameter value from the original set point.

The dimensionless sensitivity coefficient defined above enables a comparison of the sensitivities of different model parameters. As it was presented in Fig. 9, three main model parameters have a great impact on the heat flux rate: blood temperature, contact thermal resistance and thermal resistance of the plastic wall of the cooling cap channels. The first and third model parameters can be measured by carrying independent experiments. However, the second model parameter, i.e.,

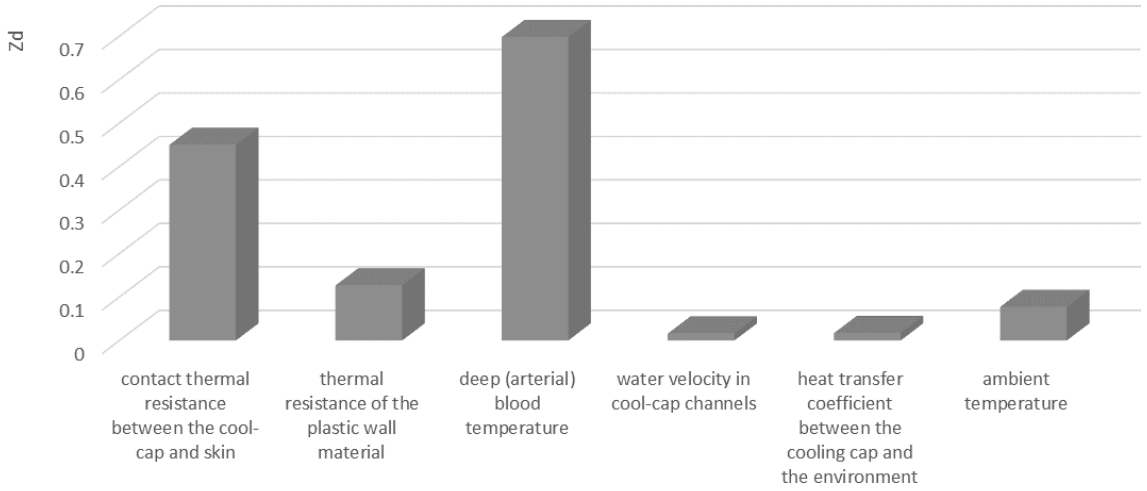

Fig. 9. Comparison of dimensionless sensitivity coefficients of the selected parameters.

the contact thermal resistance between the cooling devices and the head skin surface, is difficult to be measured and varies from case to case. This is why this particular model parameter is determined through the inverse analysis utilizing the sensitivity coefficient Z and applying the function specification function.

The *sensitivity coefficient* Z represents the first derivative of the heat flux rate with respect to the contact thermal resistance between the cooling devices and the head skin surface; therefore, it is given by:

$$Z = \frac{\partial \dot{Q}}{\partial Y_i^*}, \tag{8}$$

which can be calculated using the finite difference approximation (similarly to equation (7)):

$$Z \approx \frac{\dot{Q}\left(Y^* + \delta_Y Y^*\right) - \dot{Q}\left(Y^* - \delta_Y Y^*\right)}{\left(Y^* + \delta_Y Y^*\right) - \left(Y^* - \delta_Y Y^*\right)}. \tag{9}$$

In order to guarantee acceptable accuracy of the approximation (9), deviation of the model parameter $\delta_Y Y^*$ from the original set point Y^* needs to be appropriately small. Figure 10 presents variation of the sensitivity coefficient Z (its exact value is -155.7026 for $Y^* = 0.000413223$ was obtained from the direct model) as a function of coefficient δ_Y. It is clear from this plot that the coefficient within the range between 0.0003 and 0.0009 gives reasonable results. Hence, $\delta_Y = 0.0009$ was chosen for further calculations.

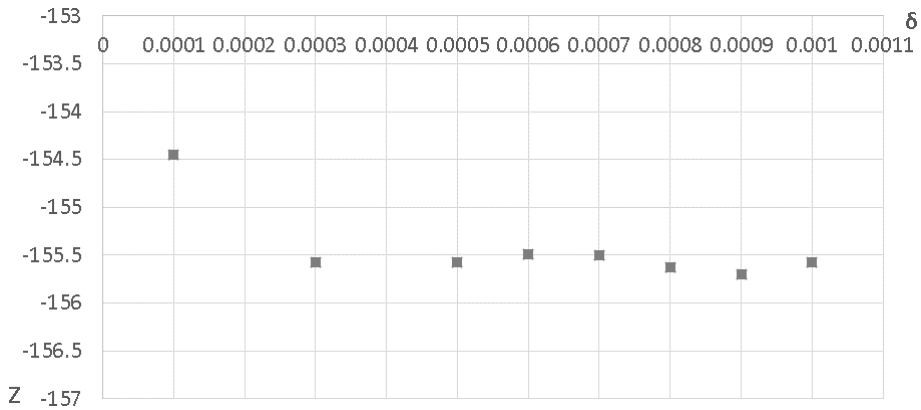

Fig. 10. Parameter deviation impact on the sensitivity coefficient value.

5. Inverse analysis

The function specification method (FSM) is an effective and widely used method to solve inverse thermal problems [10]. It was used to estimate the crucial model parameter in a sequential manner from the set of the heat flux rate measurements that are burdened with an error. Those measurements are related to one coil of the cool cap together with the appropriate part of the head, as shown in Figs 7 and 8. The FSM employs the least square methods to formulate an objective function Δ which is then minimized:

$$\Delta = \sum_{j=1}^{J} \left(\dot{Q}_j - \dot{U}_j \right)^2, \tag{10}$$

where subscript j refers to the particular measurement, J is the number of measurements, $\dot{Q}_j$ is the calculated heat flux rate while $\dot{U}_j$ is the measured heat flux rate.

The sensitivity analysis in the previous section proved that the heat flux rate is affected mostly by three model parameters. However, the analysis in this section is related to one of them, namely the contact thermal resistance.

At first, the direct problem has been solved using the set of boundary conditions with an assumed value of the contact thermal resistance equal to 0.0004132231 $\mathrm{m^2K/W}$. Since the heat flux rate $\dot{Q}_j$ transported to the water in the steady-state conditions depends on unknown contact thermal resistance, it can be expanded in a Taylor series as follows:

$$\dot{Q}_j = \dot{Q}^* + \left. \frac{\partial \dot{Q}_j}{\partial R} \right|_{R^*} (R - R^*) + \ldots, \tag{11}$$

where $\dot{Q}^*$ is a reference value of the heat flux rate, R^* is a reference value of the contact thermal resistance, $\dot{Q}_j$ is a measurement result, R is the actual value of contact thermal resistance, being estimated.

Truncating the Taylor series after the first derivative and introducing the sensitivity coefficient, the following equation can be obtained:

$$\dot{Q}_j = \dot{Q}^* + Z \left(R - R^* \right). \tag{12}$$

Finally, the value of contact thermal resistance R can be determined in the iteration process, which consists of a formula derived from (10), (11) and (12):

$$R = R^* + \frac{1}{J \cdot Z} \sum_{j=1}^{J} \left(U_j - Q^* \right). \tag{13}$$

6. Results

The value of the heat flux rate is equal to $\dot{Q}_{ex} = 1.814332$ W, calculated from the direct model, and the exact value of contact thermal resistance is $R = 0.001$ $\mathrm{m^2K/W}$ treated as the exact measurement. In order to generate real measurements $\dot{U}_j$, some errors are added to this quantity. Those errors contain randomly generated number $\varepsilon \in < 0, 1 >$ and the measurement uncertainty δ_M, i.e.,

$$\dot{U}_j = \dot{Q}_{ex} + \left(1 - 2\varepsilon_j \right) \delta_M \dot{Q}_{ex}. \tag{14}$$

Figures 11 and 12 present the results of the contact thermal resistance estimated based on the measurements burdened with an uncertainty of 2% and 1%, respectively. The more measurements are used, the more precise estimation of the parameter is obtained. The results of the 5th iteration are summarized in Tables 3 and 4.

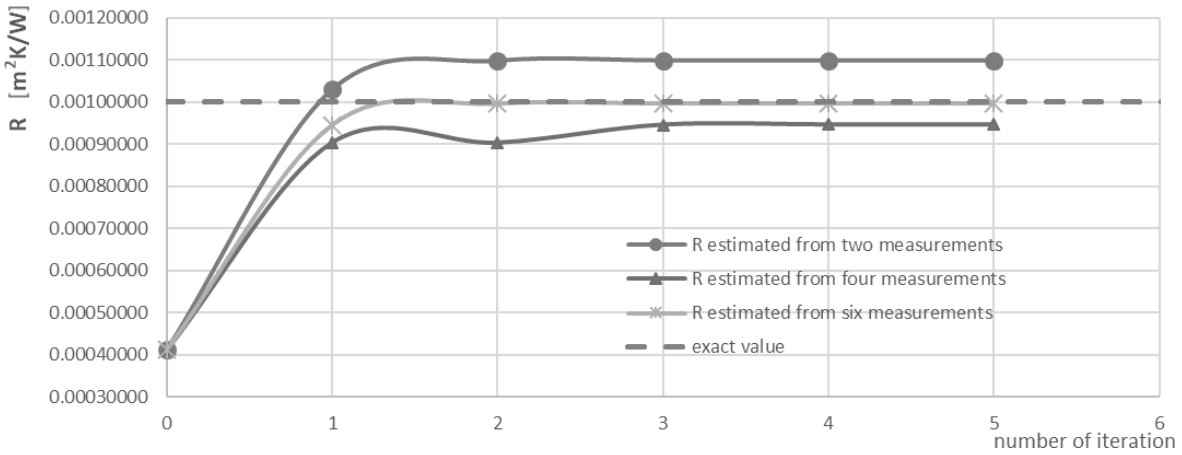

Fig. 11. Calculations based on measurements of 2% uncertainty.

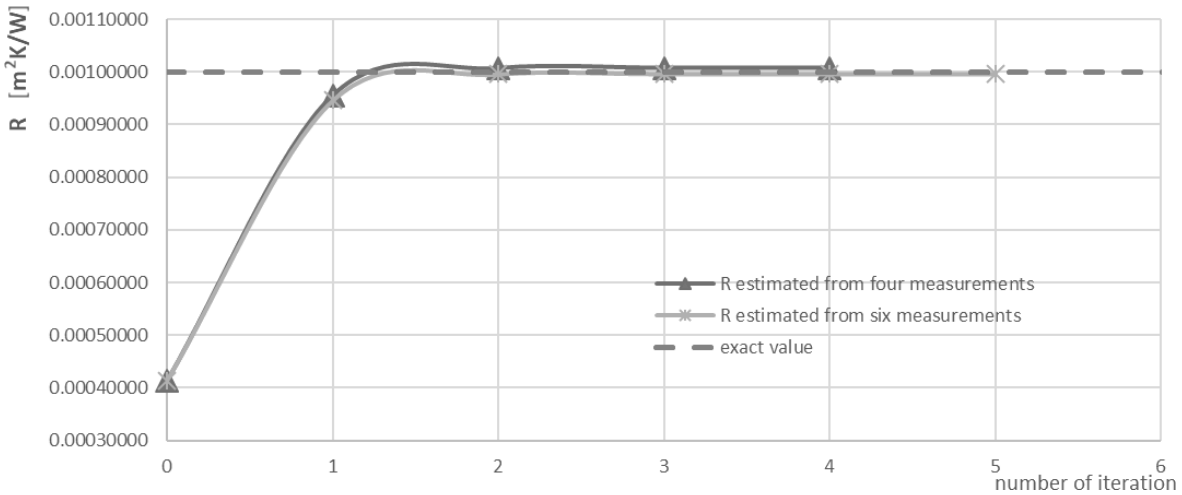

Fig. 12. Calculations based on measurements of 1% uncertainty.

Table 3. Results for calculations based on measurements of 2% uncertainty.

Measurement uncertainty	2%		
Number of measurements	2	4	6
Estimated value – contact thermal resistance [m^2K/W]	0.0010982234459	0.0009460347086	0.0009960238451
Estimation error	9.82%	–5.51%	1.57%

Table 4. Results for calculations based on measurements of 1% uncertainty.

Measurement uncertainty	1%	
Number of measurements	4	6
Estimated value – contact thermal resistance [m^2K/W]	0.0010070320070	0.0010027894442
Estimation error	0.703%	0.279%

7. Discussion

In this paper, the selective brain cooling process of the neonate and the appropriate simplified numerical model of this therapy were discussed. First of all, the sensitivities of this model on selected model parameters have been analyzed using the dimensionless sensitivity coefficients. These

analyses showed that three of them: a blood temperature, a contact thermal resistance between the cooling cap and skin of the head, and thermal resistance of the plastic wall of the cooling cap channels have a significant impact on the model results.

This paper also proposed an appropriate procedure (utilizing the FSM technique) to estimate unknown/uncertain values of the model parameters carrying out some measurements. This methodology was applied to determine a contact thermal resistance between the cooling cap and the skin of the head. Measurements were simulated by summations of the results of the direct model and randomly generated errors. The obtained results show that for more precise measurements (uncertainty of 1%), estimation error was equal to 0.7% and 0.3% for four and six measurements, respectively. The measurements with 2% uncertainty gave the estimation error equal to 9.8%, 5.5% and 1.6% when two, four, and six measurements were used, respectively. Hence, it can be concluded that the FSM procedure can be used to reduce the uncertainty of the single parameter estimation when sufficient measurement data is available.

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