PAPER • OPEN ACCESS

Thermal Design of Microreactor Structural Elements for Water Quality Analyser

To cite this article: O Matviykiv et al 2020 J. Phys.: Conf. Ser. 1534 012007

View the article online for updates and enhancements.

You may also like

- Overcoming persistent challenges in putting environmental flow policy into practice: a systematic review and bibliometric analysis Gustavo Facincani Dourado, Anna M Rallings and Joshua H Viers
- <u>Out-of-plane microvalves for whole blood</u> <u>separation on lab-on-a-CD</u> Tingjie Li, Limin Zhang, Kar Man Leung et al.
- Hydropower representation in water and energy system models: a review of divergences and call for reconciliation David E Rheinheimer, Brian Tarroja, Anna M Rallings et al.





DISCOVER how sustainability intersects with electrochemistry & solid state science research



This content was downloaded from IP address 3.137.199.182 on 14/05/2024 at 18:47

Journal of Physics: Conference Series

Thermal Design of Microreactor Structural Elements for Water Quality Analyser

O Matviykiv¹, T Klymkovych¹, I Farmaha¹, N Bokla¹, U Marikutsa¹, K Pytel²

¹Department of Computer-Aided Design Systems, Lviv Polytechnic National University, 12 Bandera Str., Lviv, Ukraine ²Department of Power Systems and Environmental Protection, AGH University of

Science and Technology, 30 Mickiewicza Al., Cracow, Poland

E-mail: matviykiv@gmail.com

Abstract. The research object is a Lab-chip device for environmental water quality monitoring. The main objective of the actual work is to determine a set of functional, geometric and technological parameters of Lab-chip microreactor to provide optimal temperature field conditions for predefined chemical reaction protocols. Since Lab-chip operates with a microdose of liquids or reagents and temperature processes in fluid flows are highly inertial, the problem of setting, maintaining and ensuring fast transient of certain temperature values in different areas of Lab-chip microchannels is nontrivial. The main focus was pointed on precise heating of defined Lab-chip areas (reaction chambers) and strict compliance with the non-stationary thermal regime, required for chemical reaction protocols. Modelling and simulation were done in COMSOL Multiphysics tool. As a result of the conducted research, there was obtained a set of parameters that provides the required thermal regime of reaction microchamber for the physicochemical determination of selected hazardous species in environmental water samples.

1. Introduction

A very broad range of modern Lab-Chip devices comprise microchambers that provide chemical reactions for the synthesis of new substances or prepares intermediate analytes for further diagnostic needs. The advances of such continuous-flow Lab-chip microreactors ensure that chemical reaction parameters like temperature, reaction rate, and reagents concentration can be precisely estimated and controlled in real-time. The extended assessment of recent laboratory and industrial microfluidic applications for direct chemical synthesis in microreactors [1], electrochemical monitoring of water hazardous impurities [2], or just water cooling of microdevices [3], has shown that all these processes can be precisely defined simply by controlling the heat and mass transfer.

Over the last decade the development, research, and optimization of Lab-chip microreactor-based devices have been carried out in several directions, like classical chemicals production systems [4], highthroughput analytical systems [5], unique instruments for the reaction kinetics study [6], in the agrofood industry [7], etc. Pharmaceutical and biomedical chemistry applications of Lab-chip microreactors with complex reaction processes and relevant biochemical synthesis have been analyzed in [8]. The review of microfluidic droplet reactors including their functional regions, like droplet generation, mixing of reactants and reaction controlling based on the mass and heat transport processes have been provided in [9]. Recently due to its enhanced performance and high effectiveness in various unit

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Published under licence by IOP Publishing Ltd 1

MicroTherm 2019 - Microtechnology and The	ermal Problem in Electronic	s	IOP Publishing
Journal of Physics: Conference Series	1534 (2020) 012007	doi:10.1088/1742	2-6596/1534/1/012007

operations, the Lab-Chip microreactor applications have been rapidly integrated into microfluidic sensors [10]. The typical Lab-chip sensor for environmental water quality monitoring system usually incorporates general multifunctional chemical microreactor. For example, the Lab-chip microchambers has been extended used for water quality analysis and phosphate monitoring [11], nitrates detection [12], various biomarkers and pollutants recognition [13], sensing of heavy metal ions in water [14], etc.

The conducted state-of-art review has shown, that effective operation of any chemical microreactor or typical Lab-chip device with reactor microchamber requires reliable thermal control. The thermal design of microfluidic devices intended to ensure the functional parameters of Lab–chip elements through the definition of an optimal set of constructive (location and sizes of microchambers), functional (heat capacity, heat transfer conditions) and technological (thermal conductivity, insulating layer) parameters, that influence the thermal regime of complete device [15]. In fact, Lab–chip for environmental water quality monitoring system is a typical multifunctional chemical microreactor, where the rates of chemical reactions strictly depend on temperature according to Arrhenius law. Thus, to determine the type and quantity of chemical components in the water sample, the temperature field of the reaction chambers and the whole Lab-chip microchannel network should be precisely controlled. In particular, the definition of nitrates/nitrites contaminants usually conducted in three stages, where the first and third reaction stages require the fixed temperature of 70°C, but much more complicated non-stationary thermal regimes are used for biochemical reactions [16]. So, the thermal design of a Lab-chip device with a deterministic temperature field is an actual task.

2. Materials and methods

The Lab-chip consists of three glass plates. The type of glass and its main properties were obtained from the COMSOL Multiphysics library. The middle plate with total dimensions of 80x50x1 mm. A complex set of microchannels for a water sample and reagents transportation was formed on the upper side of the middle plate (Figure. 1). The width of the channel is 1 mm, depth 0.4 mm, and the total length has 279 mm. Four holes were used as inlets, the last one to the right – outlet. By applied input pressure, water sample and reactants are transported into the appropriate channels (1-4), pass through the meander micromixer (6), successively enter three reaction microchambers (7-9), diagnostic chamber (10) and finally withdraw through the outlet hole (5). Each of Lab-chip inlets (1-4) may operate with different applied pressure.

On the lower side of the middle plate, there are three independent heating elements (under each reaction chamber). The heating element consists of two aluminum contacts of the size $10.0 \times 0.8 \times 0.03$ mm and an aluminum coil of 0.8 mm wide, 0.03 mm deep with a total length of 42.75 mm (11-13). Each heating element is autonomous, allowing to operate at a different voltage that gives the possibility to obtain separate temperatures in a definite reaction microchamber. A constant electric current, applied to the aluminum element due to its self-heating and constant convective boundary conditions can form an equilibrium temperature field.

The upper and lower glass plates have dimensions 80.0 x 40.0 x 1.0 mm. The supply of water sample and chemical reagents are provided through the cylindrical inlet holes with a diameter of 1.0 mm formed on the top plate.

Journal of Physics: Conference Series 1534 (2020) 012007 doi:10.1088/1742-6596/1534/1/012007



Figure 1. The layout of the Lab-chip water analyser with separate microchambers and heating elements.

In the Lab-chip microreactor, the chemical reaction characteristics (concentration, substances, time, etc.) are determined by the following parameters: the size of the reaction chamber; the fluid flow rate; the temperature distribution function over the coordinates and time.

Depending on the type of chemical reactions, it is necessary to provide different temperature values in each of the three chambers separately. Thus, appears natural requirement to minimize the spreading of the temperature field over the micro-reactor structure elements (plates, microchannels).

The temperature in the reaction microchamber depends on the following parameters [17]:

- heat capacity on the heating elements;
- size (area) of the heating element S_i , $i = 1 \dots N$, where N the number of heating elements;
- geometry and size of microchamber l_x , l_y , l_z ;
- thermal conductivity of the electro-insulating layer between heater and microchamber;
- thermal conductivity of the microchamber's material (various glass types);
- conditions of heat exchange of the microchamber with the external environment α_i ;
- heat transfer conditions (thermal conductivity) between microchamber and other Lab-chip elements (plates, microchannels).

Let us consider the processes of heat transfer in the micro-reactor elements. The heat (temperature) sources should be considered the ambient temperature T_0 and the heat flow from the heating elements. The temperature field spreads from the heating elements through the insulating layer, reagents, the chamber's wall to the external environment. We assume that the rate of the ambient temperature change is much slower than the change of the heating element temperature and can be neglected: $T_0 = const$. The typical value of ambient temperature is assumed to be in the range from 5°C up to 25°C. However, the temperature value in the microchamber depends on its own heater and the influence of heating processes in the neighboring chamber.

Consider the mathematical formalization of the presented task. The mathematical thermal model of the temperature field is defined in [18] as follows:

$$T(x, y, z, t) = W(x, y, z, t, R)$$
(1)

Where W, mathematical solution of the thermal conductivity problem in the coordinate space x, y, z, t in a restricted area; R is a vector of parameters, which includes boundary and initial conditions, geometrical sizes, thermophysical parameters of microchamber elements.

The general problem can be formulated through the method of mathematical convolution of the vector criterion and by setting restrictions for the criterion functions and the variable parameters. As a result of the vector criterion convolution we will obtain [19]:

$$Q_{i}(\overline{x}) = \sum_{i=1}^{S} w_{i} Q_{i}(\overline{x}), \qquad (2)$$

where w_i , weight coefficients that determine the importance of $Q_i(\overline{x})$. Based on the above-mentioned explanation, one can set the problem of finding the required micro-reactor parameters based on the temperature field model (1). So, as varied parameters we have to choose: x_1 , coefficient of heat transfer; x_2 , thermal flow; x_3 , temperature of external thermal actions; x_4 , coefficient of temperature conductivity. The main components of the criterion are: Q_1 - minimum or maximum of the temperature field; Q_2 - providing the functional features of the micro-reactor; Q_3 - minimum cost.

At the same time, technological constraints are applied to the thermal conductivity of the microreactor structural elements a_j , thickness h_j , and temperature drift of the chemical reaction parameters F_j . The last restriction was introduced, because of drifting temperature field values caused the temperature interaction between the neighbor microchambers. This can lead to increasing temperature instability of the chemical reaction F_m .

Mathematically, this task was formulated as follows:

$$\overline{x}^* = \{a_i^*, h_i^*\},\tag{3}$$

which provides:

Find:

$$\max_{x \in D} Q(\overline{x}) = \sum_{k=1}^{m} (T_i(\overline{x}) \max - T_k(\overline{x}) \min)^2;$$
(4)

with constraints:

$$G_{1i}(\overline{x}) = (a_i - a_i \min) (a_i \max - a_i) \ge 0; \tag{5}$$

$$G_{2i}(\bar{x}) = (h_i - h_i \min) (h_i \max - h_i) \ge 0;$$
 (6)

$$G_{3m}(\overline{x}) = (F_m^+ - F_m)(F_m - F_m^-) \ge 0, m = \overline{1, M};$$
(7)

where: $D = \{\overline{x} | \cap_{j=1}^{N} \quad G_{1j}(\overline{x}) \cap_{j=1}^{N} \quad G_{2j}(\overline{x}) \cap_{m=1}^{M} \quad G_{3i}(\overline{x})\}$, the area of an optimal solution; F_m^+, F_m^- , the borders of drift for *m*- chemical reaction parameter due to the temperature influence; *M*, the total number of controlled chemical reaction parameters.

It is rather complicated to obtain the correct analytical solution for this inverse problem, but overall temperature field distribution (1) can be obtained by using numerical methods. However, the application of decomposition methods and simplification of the above-formulated problem into partial analytical solutions does not provide the adequacy requirements for the whole model. In general, the optimal design of a multipurpose microfluidic reactor can be provided by the optimization module in CAE tools like COMSOL Multiphysics and this would increase the level of automation of the designing process.

In this research, the successful results were obtained by using a semi-heuristic approach. The initial approximation of the solution was obtained by expert conclusions. The set of variable parameters were chosen experimentally, and 67 cycles of numerical modeling experiments were conducted for various sets of parameters. The most suitable variants of layout designs of micro-reactor were analyzed and selected for prototype manufacturing.

As a solution of optimal Lab-chip design, we obtain:

thermophysical parameters of the microchambers (Figure 1.), namely thermal conductivity λ - 0.65 (chamber 7) -0.61 (chamber 8) -0.65 (chamber 9) [W / (m·K)], heat capacity at constant pressure: 4.2 · 10⁻⁴ (chamber 7) - 6.2·10⁻⁴ (chamber 8) - 4.3·10⁻⁴ (chamber 9) [J / (kg·K)], density p: 980 (chamber 7) - 992 (chamber 8) - 981 (chamber 9) [kg / m³] with thermal diffusivity a = λ / (cxp): 1.58 (chamber 7) - 0.992 (chamber 8) - 1.54 (chamber 9), which influence on the temperature interdependence between the microchamber heaters (glass is selected considering the minimum cost criterion - Q₃);

- the position of the microchambers (zero coordinate start is the left lower corner of the middle plate): the centres of the reaction chambers - (17; 15; 1.6) (chamber 7); (32; 15; 1.6) (chamber 8); (47; 15; 1.6) chamber 9) [mm], lower left corner of the diagnostic chamber - (58; 14.5; 1.6) (chamber 10) [mm];
- geometric dimensions of the chambers: reaction chambers ellipses with semi-axes of 4 and 2 [mm] respectively and 0.4 [mm] depth (chambers 7-9), a diagnostic chamber $-10.0 \times 2.0 \times 0.4$ [mm] (chamber 10);
- heat transfer conditions of the micro-reactor structure with the external environment convective heat exchange, which is determined by the equation:

$$q_0 = h \times (T_{ext} - T) \tag{8}$$

- the heat generation capacity of the heating elements (the chosen material is Al) at the current $I = 1.0 A, U = 0.25 V are q = 3.5 \cdot 103 (A V / m^2);$
- location of the heating elements (bottom left point) (Fig. 1): (14.5; 10.0; 1.0) [mm] (element 11), (29.5; 10.0; 1.0) [mm] (element 12), (44.5; 10; 1) [mm] (element 11).

The analysis of simulation results proved that non-stationary heat transfer processes in chemical Labchip microreactors are significant and should be taken into account. This allows reducing the temperature interdependence between the microchambers due to pulsed heating and a certain sequence of switching among heating elements. Next, we have taken into account the restrictions imposed by the characteristics of chemical reactions.

Let us consider the typical simulation procedure. For the designing and analysis of the Lab chip with predefined parameters, we used the interactive procedures of COMSOL Multiphysics software. The simulation gives an understanding of the overall process and allows to find new solutions, optimize constructive elements and test the Lab-chip design under different boundary conditions.

In the Lab-chip model, we use a non-isotropic single-phase laminar flow to describe the fluid flow and Joule heating to obtain the required temperature regime. Differential equations describing these processes are given in [20], where boundary conditions for all elements of the design layout are described in details. Additionally, the terms of convective heat transfer were applied to the outer Labchip boundaries and inner fluid-glass interface boundaries.

The temperature, pressure, reagent concentrations and fluid flow parameters need to be defined at the inlet holes. At this stage, the temperature of the inlet water sample was set equal to the temperature of the surrounding environment. The inlet pressure was chosen according to the direct fluid flow conditions and based on the required flow rate. For example, at pressure values of 4.0 Pa - 6.0 Pa -6.0 Pa -4.0 Pa on appropriate inlets 1-2-3-4 (Figure 1) we obtain a maximum flow rate of 1.2×10^{-4} mm/s, the average flow rate in the meander micromixer was 2.87×10^{-4} mm/s, the average flow rate in the reaction microchambers was 0.5x10⁻⁴ mm/s, 1.2x10⁻⁴ mm/s and 2.1x10⁻⁴ mm/s, respectively in microchambers 7-9, and 4.3 x 10⁻⁴ mm/s in the diagnostic microchamber 10. At the pressure values of 10.0 Pa - 14.0 Pa - 10.0 Pa, a maximum flow rate was $30.0 \times 10^{-4} \text{ mm/s}$, average flow rate in the micromixer 6×10^{-4} mm/s, average flow rate was from 2.0×10^{-4} mm/s up to 5.0×10^{-4} mm/s in the reaction microchambers, and 11.0x10⁻⁴ mm/s in the diagnostic chamber 10, respectively.

To perform Joule heating, different voltage and current settings for each heating element were applied. The predefined temperature regime in Lab-chip microchambers was set to 70°C in chamber 7, 40°C in chamber 8 and 70°C in chamber 9. Several experiments were carried out to select the geometric design of heating elements and applied electrical parameters. In particular, simulation results showed that distance between the reaction chambers has to be increased to reduce the mutual influence of their temperature fields. Also, the experiment showed that the temperature changes in the reaction chamber (under applied constant voltage) are most affected by the thickness of the heating element. So, at 1.5 V voltage and 1.0 A (heating element 11) -0.0 A (heating element 12) -1.0 A (heating element 13) during the time t = 1200 s at the thickness of the heating element 0.5 mm, the temperatures in the reaction chambers 7-8-9 were respectively 49.0°C - 33.5°C - 47.5°C. The same design, but with the heating elements thickness 0.3mm we obtained $69.0^{\circ}\text{C} - 43.0^{\circ}\text{C} - 67.5^{\circ}\text{C}$ (ambient temperature was 20.0°C).

MicroTherm 2019 - Microtechnology and	Thermal Problem in Electronics	IOP Publishing
Journal of Physics: Conference Series	1534 (2020) 012007	doi:10.1088/1742-6596/1534/1/012007

The above electrical parameters (voltage and current) are the minimum values from the allowable set, which provides the required temperature regime.

3. Results and Discussion

The result of simulation with a given configuration of the Lab-chip and the characteristics of the heating elements, current 1,0 A and voltage 1.5V on the first and third heating elements are shown in Figure 2(a). Accordingly, Figure 2(b) shows the temperature curves from 0 to 1200 s with discretion of 20 s along the straight line which goes over the top surface of the water along the channel and the reaction chambers (red line in Figure 2(a)).



Figure 2. Simulation results

It can be seen from Fig. 2(a), at t = 600 s the temperature in the first chamber is 68.40 C. At t = 900 s, the temperature rises up to 70°C and stabilizes at t = 1200 s at the value of 70.6°C.

Since the formulated inverse problem is solved ambiguously, similar temperature distribution can be obtained by selecting the electrical and structural parameters of the Lab-chip heating elements, impulse heating modes and different heat transfer conditions. For example, by reducing the thickness of the heating element, we reduce the current necessary to achieve the desired temperature, and by changing the heat exchange conditions we change the time of stabilization of the temperature field. In this way, we obtain a set of parameters that will provide a solution to the inverse task optimally.

4. Conclusions

Due to the applied semi-heuristic approach, the partial solutions of the inversed thermal design problem for the constructive elements of microfluidic Lab-chip reactor were theoretically substantiated and mathematically formulated in the proposed research. The mathematical formulation of the optimal search problem for the Lab-chip structural parameters is based on the criteria of minimum / maximum values of the temperature field, minimum manufacturing/operational expenses, and others.

The new Lab-chip device with an optimized heater system layout, dedicated to a rainwater quality monitoring system was designed and its temperature profile has been precisely investigated in the COMSOL Multiphysics.

Acknowledgments This research has been carried out within the framework of the project NAWA No PPI/APM/2018/1/00049/U/001, which is financed by the Polish National Agency for Academic Exchange.

References

[1] Elvira K, i Solvas X, Wootton R et al. 2013 The past, present and potential for microfluidic reactor technology in chemical synthesis *Nature Chemistry* **5** 905–915

[2] Jang A, Zou Z, Lee K K, Ahn C, Bishop P 2011 State-of-the-art lab chip sensors for environmental water monitoring *Measurement Science and Technology* **22** 1-18

IOP Publishing

Journal of Physics: Conference Series

1534 (2020) 012007 doi:10.1088/1742-6596/1534/1/012007

- [3] Raj E, Lisik Z, Langer M, Tosik G, Wozny J 2005 The numerical approach to analysis of microchannel cooling systems *Lecture Notes in Computer Science* **3514** 876-883
- [4] Jensen K F, Reizman B J, Newman S G 2014 Tools for chemical synthesis in microsystems *Lab Chip* **14** 3206–3212
- [5] Gómez-Hens A, Fernández-Romero J 2017 Microfluidic Systems in Analytical Chemistry *Encyclopedia of Analytical Chemistry* 1-20.
- [6] Chao Liu, Ying Li, Bi-Feng Liu 2019 Micromixers and their applications in kinetic analysis of biochemical reactions *Talanta* **205** 120-136
- [7] Kim G, Lim J, Mo C 2016 Applications of Microfluidics in the Agro-Food Sector: A Review *Journal of Biosystems Engineering* **41(2)** 116-125
- [8] Liu D, Cito S, Zhang Y et al. 2015 A versatile and robust microfluidic platform toward high throughput synthesis of homogeneous nanoparticles with tunable properties *Advanced Materials* 27 2298–2304
- [9] Liang-Jun Pan, Jia-Wei Tu, Hao-Tian Ma et al. 2018 Controllable synthesis of nanocrystals in droplet reactors *Lab on a Chip* **18** 41-56
- [10] Suryawanshi P, Gumfekar S, Bhanvase B, et al. 2018 A review on microreactors: Reactor fabrication, design, and cutting-edge applications *Chemical Engineering Science* **189** 431–448
- [11] Clinton-Bailey G S, Grand M M, Beaton A D et al. 2017 A lab-on-chip analyzer for in situ measurement of soluble reactive phosphate: improved phosphate blue assay and application to fluvial monitoring *Environmental Science & Technology* **51** 9989-9995
- [12] Alahi M E E, Mukhopadhyay S C 2018 Detection methods of nitrate in water: A review *Sensors* and Actuators A: Physical **280** 210–221
- [13] Piaskowski K, Świderska-Dąbrowska R, Kaleniecka A, Zarzycki P K 2017 Advances in the Analysis of Water and Wastewater Samples Using Various Sensing Protocols and Microfluidic Devices Based on PAD and μTAS Systems, *Journal of AOAC International* **100(4)** 962-970
- [14] Li S, Zhang C, Wang S, Liu Q et al. 2018 Electrochemical Microfluidics Techniques for Heavy Metal Ions Detection Analyst 143(18) 4230-4246
- [15] Streit P, Nestler J, Shaporin A, Schulze R, Gessner T 2016 Thermal Design of Integrated Heating for Lab-On-A-Chip Systems Proc. 17th International Conference on Thermal Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems (EuroSimE) 2016 Montpellier 1-6
- [16] Martinez-Quijada J, Ma T, Hall G H, et al 2015 Robust thermal control for CMOS-based lab-onchip systems *Journal of Micromechanics and Microengineering* **25**(7) 1-13
- [17] Yang F, Yang N, Huo X, Xu S 2018 Thermal sensing in fluid at the micro-nano-scales *Biomicrofluidics* 12(4) 1-32
- [18] Lobur M, Farmaga I, Marikutsa U, Matviykiv O, Ciupinski L 2011 Analysis and problem statement of the optimal thermal design of technical objects *Proc. International Conference on Microtechnology and Thermal* 2011 Lodz Poland 223-227
- Batishchev D 1979 Tasks and Methods of Vector Optimization Gorkiy University Press 1-92 (In Russian)
- [20] Matviykiv O, Klymkovych T, Bokla N, Farmaha I, Pytel K 2019 Design and Analysis of Lab-Chip Module for Rainwater Chemical Hazards Monitoring System Proc. International Conference on the Experience of Designing and Application of CAD Systems 2019 Polyana Ukraine 1-4