Modeling and analysis of energy efficiency of methods for maintaining temperature conditions in microbioreactors

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Abstract. A mathematical model of maintaining the thermal conditions of microreactors used in biological, medical and other experiments that require stabilization or temperature control software is considered. Several heating modes are considered: using a liquid heating jacket, heating from below through the bottom, heating from the side using a flexible silicone heater. Simulated heat loss and dynamic modes of temperature control.

Introduction

Providing the required temperature conditions during the operation of reactor vessels during biological, chemical or medical experiments is a guarantee of valid and repeatable results. As a rule, various types of heaters are used to ensure the set temperatures: heating tiles, shirts, or flexible heaters fixed to the wall of the reactor.

The aim of the work is to select the optimal quality control structure for energy and energy efficiency to maintain the given temperature of the microreactor, which is planned to be used when conducting experiments in the framework of SHIME type models [1].

1. Methods and models

For research, we will use methods of mathematical modeling of the object using ordinary differential equations (ODE) [2], computer simulation [3] and verification of the results obtained on the experimental layout of the microreactor temperature stabilization system.

1.1 Mathematical model of a microreactor based on a glass container, basic version

Consider a cylindrical tank with known geometric and physical parameters, filled with liquid to a level $h$ (figure 1).

The mathematical model of the thermal regime of the microreactor is created using the method of storage and flows (for example, [4]) and in the basic version (only for the microreactor itself) has the form:

$$\frac{d\vartheta_h}{dt} = \frac{1}{\rho_h \cdot V_h \cdot c_h} \left( G - S \left( \alpha_0 + \alpha_1 \vartheta \right) \left( \vartheta_h - \vartheta_g \right) \right)$$

$$\frac{d\vartheta_g}{dt} = \frac{1}{\rho_g \cdot V_g \cdot c_g} \left( S \left( \alpha_0 + \alpha_1 \vartheta \right) \left( \vartheta_h - \vartheta_g \right) - S \left( \alpha_2 + \alpha_3 \vartheta_{ext} \right) \left( \vartheta_g - \vartheta_{ext} \right) \right)$$

(1)

The model parameters are shown in Table 1. The values of the physical constants are taken from [5].
| Designation | Dimension | Value | Note |
|-------------|-----------|-------|------|
| $b$         | m         | 0.06  | Base diameter |
| $h$         | m         | 0.08  | Chyme level height |
| $d$         | m         | 0.001 | Wall thickness |
| $\rho_h$    | kg/m$^3$  | 1000  | Chyme density |
| $c_h$       | J/(kg*K)  | 4200  | Heat capacity of chyme |
| $\alpha_0$  |           | 450   | stat. part of water-to-surface heat transfer coefficient |
| $\alpha_1$  |           | 2100$\sqrt{v}$ | dyn. part of water-to-surface heat transfer coefficient |
| $\alpha_2$  |           | 5.6   | stat. part of air-to-surface heat transfer coefficient |
| $\alpha_3$  |           | 4$\times v$ | dyn. part of coefficient water-to-surface heat transfer |
| $\lambda$   | W/(m*K)   | 1.2   | Thermal conductivity of Pyrex glass |
| $\rho_g$    | kg/m$^3$  | 2230  | Pyrex glass density |
| $c_g$       | J/(kg*K)  | 830   | Heat capacity of Pyrex glass |
| $V_g$       | m$^3$     | $(\pi \cdot b^2 / 4 + 2 \cdot \pi \cdot b \cdot h) \cdot d$ | Pyrex glass volume |
| $V_h$       | m$^3$     | $\pi \cdot h \cdot b^2 / 4$ | Chyme volume |
| $S_1$       | m$^2$     | $2 \pi \cdot b \cdot h$ | The contact area of the chyme with the walls of the glass |
| $S_2$       | m$^2$     | $\pi \cdot b^2 / 4$ | The contact area of the chyme with the bottom of the glass |
| $v_h$       | m/c       | 0.01  | The speed of the chyme along the wall |
| $v_g$       | m/c       | 0.01  | Air velocity along the wall |
| $G$         | W         | 5     | Heat flow from heater, max. |
| $\theta_{ext}$ | °C       |       | Ambient temperature |
| $\theta_h$  | °C        |       | Chyme temperature |
Figure 1. Objects of modeling. “a” – model with inherent heating (1), “b” – model with bottom heating (2), “c” – model with side heating (3)

The model of the dynamic system (1) has the following structure (figure 2)

\[
\frac{d\theta_h}{dt} = \frac{1}{\rho_h \cdot V_h \cdot c_h} \left( S_{p} \lambda_p (\theta_p - \theta_h) - S (\alpha_0 + \alpha_1 v) (\theta_h - \theta_g) \right)
\]

\[
\frac{d\theta_g}{dt} = \frac{1}{\rho_g \cdot V_g \cdot c_g} \left( S(\alpha_0 + \alpha_1 v_h)(\theta_h - \theta_g) - S(\alpha_2 + \alpha_3 v_{ext})(\theta_g - \theta_{ext}) \right)
\]

\[
\frac{d\theta_p}{dt} = \frac{1}{m_p \cdot c_p} \left( G - S_{c} \lambda_p (\theta_p - \theta_h) \right)
\]

Figure 2. The structure of the model of microreactor with internal heating.

1.2. Mathematical model of a microreactor based on a glass tank, heated from bottom

Consider the model of a microreactor heated from below using a classic heater with a magnetic stirrer. In this case, the dynamics of heating will change due to the appearance of another inertial system.
Additional parameters corresponding to the characteristics of the heater are given in Table 2.

**Table 2. The model (2) additional parameters**

| Designation | Dimension | Value | Note |
|-------------|-----------|-------|------|
| $m_p$       | kg        | 0.3   | Heater mass |
| $c_p$       | J/(kg*K)  | 900   | Heat capacity of heater (Al) |
| $\lambda_p$ | W/(m*K)   | 500   | Coeff. heat transfer from the heater to glass |

The model of the dynamic system (2) has the following structure (figure 3)

**Figure 3. The structure of the model (2) of microreactor with external (bottom) heating**

1.3. *Mathematical model of a microreactor based on a glass tank, side heating*

For a silicone film heater located on the side wall of a microreactor, the model takes the following form:

\[
\begin{align*}
\frac{d\vartheta_h}{dt} &= \frac{1}{\rho_h \cdot V_h \cdot c_h} S_1 \alpha_h (\vartheta_h - \vartheta_s) \\
\frac{d\vartheta_g}{dt} &= \frac{1}{\rho_g \cdot V_g \cdot c_g} \left( S_1 \lambda_p \left( \vartheta_p - \vartheta_g \right) - S_2 \lambda_p \left( \vartheta_h - \vartheta_g \right) \right) \\
\frac{d\vartheta_{p1}}{dt} &= \frac{1}{m_{p1} \cdot c_{p1}} \left( G - S_1 \lambda_p \left( \vartheta_p - \vartheta_g \right) - S_1 \alpha_1 \left( \vartheta_g - \vartheta_{ext} \right) \right)
\end{align*}
\]
Additional parameters corresponding to the characteristics of the heater are given in Table. 3

### Table 3. The model (3) additional parameters

| designation | dimension | value | note |
|-------------|-----------|-------|------|
| $m_p$       | kg        | 0.03  | Heater mass |
| $c_p$       | J/(kg*K)  | 1.420 | Heat capacity of heater (Al) |
| $\lambda_p$ | W/(m*K)   | 500   | Coeff. heat transfer from the heater to glass |

The model of the dynamic system (3) has the following structure (figure 4)

![Figure 4](image_url)

**Figure 4.** The structure of the model (3) of microreactor with external (side) heating

In this case, the mass of the heater is significantly reduced, reducing its inertia, and the contact area of the heater with the capacity (and chyme) increases.

### 2. Results of simulations

A computer study of the dynamics of a microreactor based on the above mathematical models was carried out in the mathematical package Matlab.

The simulation result of heating the microreactor with an abstract heater emitting 5 Watts of power inside the chyme is shown in figure 5

![Figure 5](image_url)

**Figure 5.** Dynamics of heating a microreactor with internal heating (model (1)) at $P = 5$ W
Adding a PI-controller to the model allows you to provide a given temperature when the temperature of the environment with an amplitude of 2 °C. Obtained results shown in fig. 6.

**Figure 6.** Dynamics of the temperature of a microreactor (model (1)) with a temperature of 36 °C: “a” for a constantly external temperature, “b” for a sinusoidally changing temperature.

For PI-controller parameters \( k_p = 20 \), \( k_i = 0.1 \), the following graphs were obtained for model (2) (figure 7).

The simulation results of the dynamics of heating the microreactor on the side (model (3)) with the same parameters of the PI controller are shown in figure 8. By reducing the inertia of the heater, the dynamics of the system changes positively.
3. Experimental layout
To compare the results of computer simulation with the heating of a real microreactor, an experimental model was developed that included a laboratory machine as a microreactor, a microprocessor control system, and a laptop computer for recording the results (figure 9). The structure of the microprocessor control system is shown in figure 10. As the control controller, Arduino UNO was used, in the program of which a digital controller and a PWM controller for controlling the heater were implemented. To measure the chyme temperature and external temperature, digital thermometers of the DS18B20 type [6] with a 1-Wire interface were used. Some decisions were borrowed from [7].

**Figure 7.** Dynamics of the temperature of a microreactor (model (2)) with a temperature of 36 °C

**Figure 8.** Dynamics of the temperature of a microreactor (model (3)) with a temperature of 36 °C
To ensure heating, a flexible heater in a silicone case was used, covering approximately 50% of the microreactor wall. Heater power is 5 watts.

During the experiment, the measurement results (chyme temperature, ambient temperature, current consumed by the heater) were transferred via a serial interface to a portable computer, and saved to a file. The measurement results are shown in figure 11 against the background of the results of simulation modeling of model (3) under the corresponding initial and external conditions.

![Figure 9. Appearance of the laboratory layout. "a" is the system as a whole, "b" is a microreactor simulator](image)

![Figure 10. The structure of the microprocessor control system](image)

![Figure 11. The measurement results (points & blue line) against the background of the results of simulation modeling of model (3) (green line)](image)
4. The discussion of the results
Three mathematical models of heating a microreactor were developed and investigated by computer simulation methods: with ideal heating in the volume of the chyme, with heating from the bottom and heating from the side of the side wall. A digital controller was included in the model, which was supposed to provide stabilization of the chyme temperature at a given level. The simulation results presented in figure 11 showed that the system with side heating is closer in characteristics to the ideal model, and on this basis, it can be recommended for implementation.

During the study of the models, the total energy spent on maintaining the set temperature in each of the cases was estimated, it is given in table 4 and illustrated in figure 12.

Table 4. The total energy spent of different models

| Models  | Energy, J |
|---------|-----------|
| Model (1) | 53419.66 |
| Model (2) | 56623.92 |
| Model (3) | 55063.93 |

Figure 12. Histogram of total energy spent of different models

Based on the data obtained, it can be argued that according to the energy criterion, a model with side heating (model (3)) is preferable to a model with heating through the bottom (model (2)). Figure 13 shows comparative graphs of the control action on the model, with a sinusoidal change in external temperature. In this case, model (3) (red line) is also closer to the ideal model (1) (green line).

Figure 13. Comparative graphs of the control action on the model, with a sinusoidal change in external temperature
Conclusions
In order to verify the system’s operability in practice, an experiment was conducted to heat the chyme simulator (water) using a flexible heater, and the results (figure 11) showed good qualitative and good quantitative agreement with the simulation results. Some discrepancy in the operation of the digital controller is possible due to its simplified implementation in the microcontroller, compared to Matlab. The results obtained made it possible to justify the choice of lateral heating as the most suitable for implementation in the system of maintaining the temperature regime of the microreactor for biological and medical experiments.

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