



Theoretical and fuzzy modelling of a pharmaceutical batch reactor

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ABSTRACT

This paper deals with the development of a batch-reactor model with a theoretical and a locally affine fuzzy model. The batch reactor is used in the pharmaceutical industry for the production of drugs, where a rapid and precise temperature control is necessary. The model has to be built to include all the main features necessary for the purposes of modelling. The development of the model for the reactor is designed for further control development and simulation purposes, without doing any further experiments on the real process. In our case we use the model for simulating the reactor's jacket temperature and the reactor's core temperature. The theoretical model describes all the nonlinearities of the process of heating and cooling the content of the batch reactor. The main contribution of the theoretical model is in the modelling of the heat transfer between the reactor's jacket and the reactor's core, mainly caused by the change in the overall heat transfer, which also covers the main nonlinearity. Because of the complexity of the theoretical model a locally affine fuzzy model is also developed.

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1. Introduction

This paper deals with the development of a theoretical and a locally affine fuzzy model for the process of heating and cooling the content of a reactor. Since the modelled reactor is used for the preparation of solvents added to the production of active pharmaceutical substances, a rapid and precise temperature control of the reactor's content is essential. Drastic changes in the prescribed temperature, the various uses of the reactor, the mixed continuous and discrete hybrid nature of the process's behaviour and the equipment require good control. For this reason a conventional PID controller is ineffective for the entire operating range. To improve the performance of the temperature control of the reactor's contents a good model of the reactor is needed for further control development and simulation purposes. The control depends on the choice of the discrete heating–cooling medium and the position of the continuous analog valve. We are therefore dealing with a hybrid nonlinear system. The progress and the challenges in batch-process control are presented in [1,2].

In the literature a number of papers and books have been published that discuss the construction of a theoretical model. The basic theoretical models of a batch reactor were, for example, described in [3–7]. These books and articles contain theoretical models for different types of batch reactors and the basis of the heat conduction between the reactor's jacket, the reactor's core and to the reactor's surroundings. The main contribution of our theoretical model is in the modelling of the heat transfer between the reactor's jacket and the reactor's core, mainly caused by the change in the overall heat transfer, as proposed in [8–10], which also covers the main nonlinearity. In these books different methods for the calculation of the overall heat transfer between the reactor's jacket and the reactor's core are presented. In our case the best way to cover the nonlinearities of the overall heat transfer is by a correlation equation given by Petukhov in [11].

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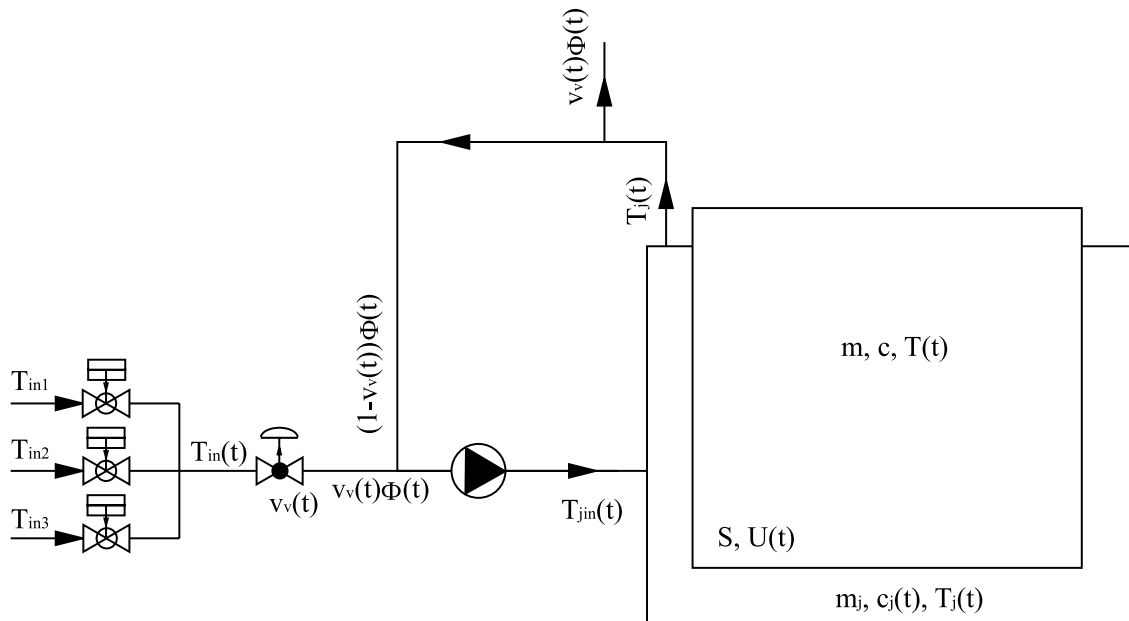


Fig. 1. Scheme of the reactor.

For developing and testing control algorithms for the temperature control of the reactor's content we build a locally affine fuzzy model because the theoretical model is too complex. The local linear models are built on the basis of the theoretical model. In our case this is done by using the Takagi–Sugeno fuzzy model proposed by [12–17] with the fuzzification of the nonlinear parameters as described in [18].

The paper is organized in the following way: Section 2 contains the construction of the batch reactor, Section 3 contains a detailed theoretical model for the heating and cooling of the reactor's content, Section 4 contains a comparison between the measurements taken on the real process and the theoretical model, Section 5 contains the derivative of a locally affine fuzzy model, and the last section contains a comparison between the simulation on the theoretical model and the locally affine fuzzy model.

2. The construction of the batch reactor

The modelled reactor is made of stainless steel and serves for the preparation of solvents that are added to the production of drugs. The capacity of the reactor is 630 litres. The heating and cooling of the reactor's content is via pipes in the form of coils that are wrapped around the wall of the reactor. Through these pipes flows a heating–cooling medium (a mixture of water and glycol) that is at three different temperatures: 140, 5 and -25 °C. Depending on the desired temperature, we use one of the three possible medium mixtures to heat or cool the reactor's core. The medium mixture with the right temperature is set by the position of three on/off valves. The medium flows via the adjustable analog valve, with the help of a pump, into the reactor's jacket. The modelling of the reactor's temperature is a nonlinear process that depends on several input parameters. As described in [4,9,2] the rate of changing the reactor's temperature is affected by the following parameters:

- the choice of the input heating–cooling medium;
- the position of the analog valve;
- the mass of the mixture in the reactor;
- the heat capacity of the mixture;
- the heat capacity of the heating–cooling medium;
- the thermal conductivity between the reactor's core and the jacket;
- the conduction surface;
- the temperature of the reactor's jacket.

The speed of the reactor's mixer has only a minimal impact on change of the temperature in the reactor's core. The speed must reach a point at which the temperature around the reactor's content stays the most constant. The peristaltic pump operates with a constant power and pumps the heating–cooling medium through the reactor's jacket.

A scheme of the reactor is shown in Fig. 1. The reactor's temperature T is regulated by the jacket inlet temperature T_{jin} and the reactor's jacket temperature T_j . The reactor's jacket is made of tubes forming a coil that is wrapped around the wall of the reactor's core. By building the reactor's model we simplify the jacket as a flat plate connected to the reactor's core with

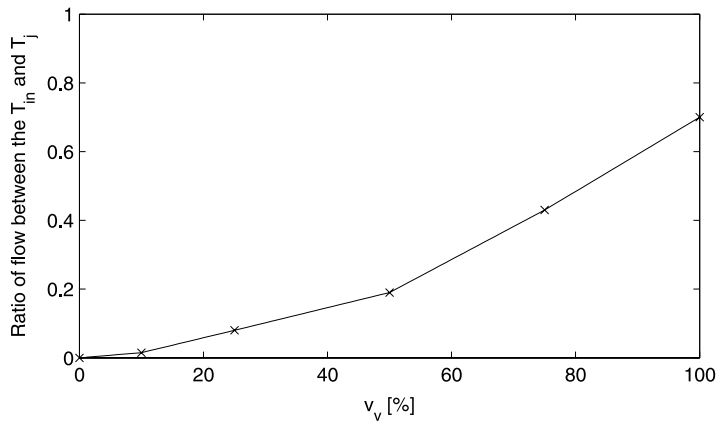


Fig. 2. Characteristic of the analog valve.

Table 1

Characteristics of the water–glycol (50%–50%) mixture.

Temperature (°C)	–25	–17.8	4.4	26.7	48.9	71.1	93.3	138
Viscosity (kg/ms) · 10 ^{–3} – μ	45	22	6.5	2.8	1.5	0.9	0.7	0.6
Heat capacity (J/kg K)– c_p	3250	3265	3327	3411	3482	3558	3621	3762
Flow (l/s)– Φ	3.7	/	3.87	4.06	/	4.1	/	4.14
Thermal conductivity (W/mK) · 10 ^{–3} – λ_{medium}	415	414	409	404	398	385	371	355

the surface S . The heat transfer between the reactor's core and the jacket is defined by the overall thermal conductivity U . For the purpose of the model's construction we presumed that the reactor is filled with water with mass m and heat capacity c . The mass of the water in the reactor may vary, and because the reactor's jacket is isolated with an 8 cm thick layer of glass wool, we can ignore the heat passing through the isolation. The heating–cooling medium that flows through the jacket is a mixture of glycol and water 50%–50% (m_j , c_j). The pump pushes the heating–cooling medium with the constant flow Φ . For the heating and cooling of the reactor's core we use three discrete input heating–cooling mediums, which cannot be mixed. The choice of the medium is determined by opening the on/off valve for the chosen medium at the temperature T_{in} : $T_{in1} = -25$ °C, $T_{in2} = 5$ °C, $T_{in3} = 140$ °C. The position of the analog valve v_v provides the flow for the selected heating–cooling medium. The flow of the heating–cooling medium into the reactor's jacket provides its temperature and consequently heats up the reactor's content. Our developed model will be used to control the temperature of the reactor's content by choosing the heating–cooling medium T_{in} and the position of the analog valve v_v . The characteristic of the analog valve is not known a priori; we obtain it by comparing the simulation results of the theoretical model and the measurements made on the reactor. The characteristic of the analog valve is shown in Fig. 2.

3. Theoretical model

The theoretical model is defined by the first law of thermodynamics, the conservation of energy, described in the following equations:

$$T_{jin}(t) = v_v(t)T_{in}(t) + (1 - v_v(t))T_j(t) \quad (1)$$

$$\frac{dT_j}{dt} = \frac{\Phi(t)}{m_j} T_{jin}(t) - \left(\frac{\Phi(t)}{m_j} + \frac{U(t)S}{m_j c_j(t)} \right) T_j(t) + \frac{U(t)S}{m_j c_j(t)} T(t) = f_1(T_{jin}, T_j, T) \quad (2)$$

$$\frac{dT}{dt} = \frac{U(t)S}{mc} T_j(t) - \frac{U(t)S}{mc} T(t) = f_2(T_j, T). \quad (3)$$

By studying the process of heating and cooling of the reactor's contents we can establish that it is not linear in terms of its parameters. The overall thermal conductivity between the reactor's core and the reactor's jacket varies as a function of the temperature change in the reactor's jacket. The thermal conductivity change is most affected by the viscosity (μ – Table 1), as given in [19], of the heating–cooling water. A higher viscosity means that a thick film of the heating–cooling medium is formed on the walls inside the tubes, which reduces the thermal conductivity. The pressure of the heating–cooling medium is under 4 bars, which allows a higher boiling point for our mixture of water and glycol. Otherwise the mixture would start to boil at 140 °C. The overall thermal conductivity is also affected by the change in the thermal conductivity of stainless steel, which depends on the wall thickness between the reactor's jacket and the reactor's core (λ – Table 2), as described in [20], as well as on the specific heat and the thermal conductivity of the heating–cooling medium (c_p and λ_{medium} – Table 1), as given in [19]. The change of the viscosity of the heating–cooling medium also affects this flow (Φ – Table 1).

Table 2
Thermal conductivity of the stainless steel type AISI 316.

Temperature (°C)	–73	27	127	227
Thermal conductivity (W/mK)— λ	11.2	13.2	15.2	16.75

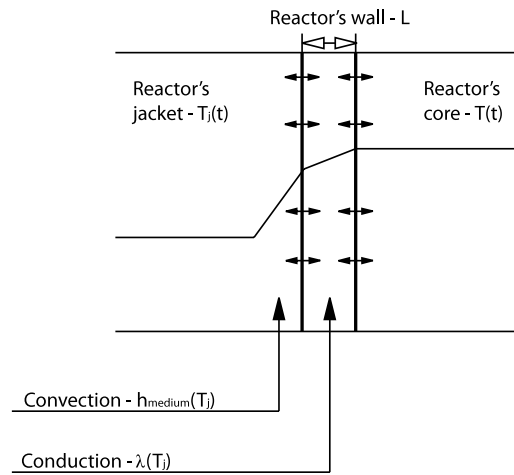


Fig. 3. Thermal conductivity over the flat plate.

As mentioned the reactor's content is heated–cooled via pipes in the form of coils that are wrapped around the wall of the reactor. The overall thermal conductivity between the reactor's core and the reactor's jacket can be simplified and represented as forced thermal convection and conduction through a flat plate, as proposed in [10], shown in Eq. (4) and Fig. 3.

$$\frac{1}{U} = \frac{1}{h_{\text{medium}}} + \frac{L}{\lambda}. \quad (4)$$

Here, L is the thickness of the reactor's wall, λ is the thermal conductivity of the stainless steel and h_{medium} is the forced thermal convection through a flat plate, described by a correlation given by Petukhov in the following equation, as in [11].

$$h_{\text{medium}} = \frac{\lambda_{\text{medium}}}{L_{\text{conv}}} \frac{0.037\text{Re}^{0.8}\text{Pr}}{(1 + 2.443\text{Re}^{-0.1}(\text{Pr}^{0.67} - 1))}, \quad (5)$$

where λ_{medium} is the thermal conduction of the heating–cooling medium, L_{conv} is the characteristic length of the heat convection, Pr is the Prandtl number and Re is the Reynolds number. From this it follows:

$$\text{Pr} = \frac{\mu c_j}{\lambda_{\text{medium}}} \quad \text{and} \quad \text{Re} = \frac{L_{\text{conv}} V \rho}{\mu}, \quad (6)$$

where

$$\rho = \rho_{\text{water}}/2 + \rho_{\text{glycol}}/2 \quad \text{and} \quad V = \Phi/S_{\text{tube}} = \Phi/\pi r_{\text{tube}}^2 \quad (7)$$

and where

- $r_{\text{tube}} = 0.03$ m is the radius of the tube forming the reactor's jacket;
- $L_{\text{conv}} = 11.37$ m is the length of the pipe wrapped around the reactor;
- $\rho_{\text{water}} = 1000$ kg/m³ is the specific gravity of water;
- $\rho_{\text{glycol}} = 1096$ kg/m³ is the specific gravity of glycol;
- $\rho = 1048$ kg/m³ is the specific gravity of the mixture of water and glycol;
- $S = 3$ m² is the heat-exchanging surface;
- $c = 4186$ J/kg K is the heat capacity of the water;
- $m_j = 120$ kg is the mass of the heating–cooling medium in the reactor's jacket and its circulation;
- $L = 0.017$ m is the thickness of the wall between the reactor's core and the reactor's jacket.

Using the above equations and the data on our process, we can calculate the overall thermal conductivity between the reactor's core and the reactor's jacket at different temperatures of the heating–cooling medium and the steel.

Table 3
Input parameters for the measurements made on the reactor.

Time (min)	0:00	7:50	31:15	42:00	54:10	59:30	65:40	80:30	127:30
Mass of water in reactor (l) – m	630	630	630	630	615	615	615	615	615
Heating–cooling medium ($^{\circ}\text{C}$) – T_{in}	5	140	140	140	5	5	5	–25	5
Position of the valve (%) – v_v	100	50	25	75	100	50	100	100	100

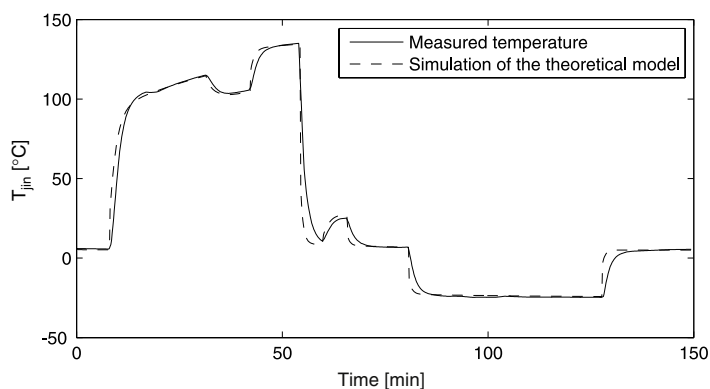


Fig. 4. Jacket's inlet temperature: measured and simulated.

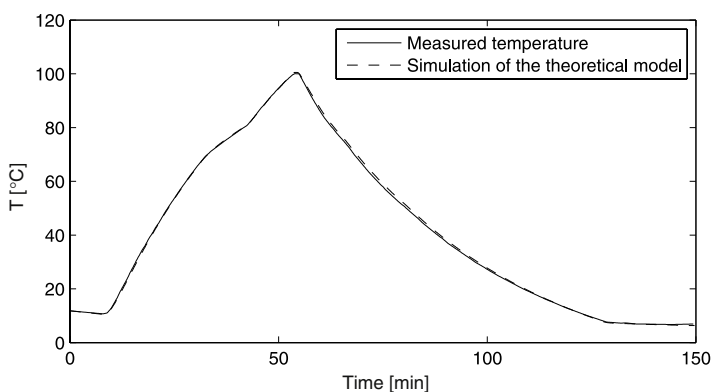


Fig. 5. Reactor's core temperature: measured and simulated.

4. Validation of the theoretical model

In this section the simulation results of the theoretical model are compared to the measurements made on the real process. The input parameters for the theoretical model are listed in Table 3.

- The choice of the heating–cooling medium is determined by the partial opening of the three on/off valves. They have two possible states: open and closed. Mixing of the heating–cooling medium at three different input temperatures is not possible. Only one on/off valve can be open at a time.
- The position of the analog valve is between 0% and 100% and defines the flow of the input heating–cooling medium.
- As the reactor is being used for the preparation of solvents with a low viscosity we can fill the reactor with water.

Comparisons between the simulation results of the theoretical model and the measurements taken on the real process are shown in Figs. 4 and 5. While Fig. 4 shows a comparison of the simulation results and the measurements of the temperature of the reactor's jacket, Fig. 5 shows the comparison of the simulation results and the measurements for the reactor's core temperature.

The accuracy of the theoretical model is measured with the root mean square deviation between the simulated and measured temperatures for the reactor's jacket (Eq. (8)) and the reactor's core (Eq. (9)).

$$RMSD_j = \frac{\sqrt{\sum_{i=1:n} (T_{jin, simulated}(i) - T_{jin, measured}(i))^2}}{n}, \quad (8)$$

$$RMSD = \frac{\sqrt{\sum_{i=1:n} (T_{\text{simulated}}(i) - T_{\text{measured}}(i))^2}}{n}, \quad (9)$$

where n is the number of the measurements – simulation points.

The deviation for the reactor's jacket is $RMSD_j = 3.04$ °C and for the reactor's core is $RMSD = 0.34$ °C.

5. Locally affine fuzzy model

The theoretical model for the process of heating and cooling the reactor's content, described in Section 3, is nonlinear in the parameters. To approximate the nonlinearities of the process we use the fuzzy formulation. Fuzzy models can be regarded as universal approximators, which can approximate continuous nonlinear processes to an arbitrary precision [17].

The locally affine fuzzy model is a set of local linear models that are different in terms of parameters and depend on the operating point. The proposed fuzzy model is described in [21]. The rules R^j describe the fuzzy model as proposed by the Takagi–Sugeno fuzzy model [15] and are given in Eq. (10).

$$R^j() : \\ \text{IF } x_1 \text{ is } A_1^j \text{ and } \dots \text{ and } x_i \text{ is } A_i^j \text{ and } \dots \text{ and } x_n \text{ is } A_n^j \text{ THEN } y_j = f_j(x_1, \dots, x_n) = a_{1j}x_1 + \dots + a_{nj}x_n + r_j \\ a_{1j}, \dots, a_{nj}, r_j \in \mathfrak{R}, \text{ FOR } j = 1, \dots, K \quad (10)$$

Here, A^j is the antecedent fuzzy set of the j th rule that is associated with a real-valued function $\mu_{A_i^j} : \mathfrak{R} \rightarrow [0 \ 1]$, that produces the membership grade. a_{nj} are the parameters of the polynomials and r_j is the offset parameter. The parameter K defines the number of rules in the model. The system in the above equation can be described in closed form if the intersection of the fuzzy sets is previously defined. The generalized form of the intersection, determined with sharpening, uses the T -norm as proposed in [22]. According to the rules R^j and the appropriate membership functions $\mu_{A_i^j}$ is the output defined in Eq. (11).

$$y = \sum_{j=1}^K \frac{\prod_{i=1}^n \mu_{A_i^j}}{\sum_{j=1}^K \prod_{i=1}^n \mu_{A_i^j}} y_j \quad (11)$$

The dynamics of the reactor's temperature control is described by the theoretical model. By building a locally affine fuzzy model we consider all of its nonlinearities. The locally affine fuzzy model is obtained from the linearized nonlinear model at a specific operating point. For the linearization of the reactor's dynamics we have to derive the equations by the variables, which affect the temperature in the reactor's jacket (Eqs. (12) and (13)) and the reactor's core (Eqs. (14) and (15)).

$$f_1(T_{jin}, T_j, T) \approx \left. \frac{\partial f_1}{\partial T_{jin}} \right|_{T_{jin}, T_j, T} T_{jin} + \left. \frac{\partial f_1}{\partial T_j} \right|_{T_{jin}, T_j, T} T_j + \left. \frac{\partial f_1}{\partial T} \right|_{T_{jin}, T_j, T} T \quad (12)$$

$$f_1 = \frac{\Phi}{m_j} T_{jin} - \left(\frac{\Phi}{m_j} + \frac{S}{m_j c_j} \frac{\partial U}{\partial T_j} T_j + \frac{US}{m_j c_j} - \frac{S}{m_j c_j} \frac{\partial U}{\partial T} T \right) T_j + \frac{US}{m_j c_j} T \quad (13)$$

$$f_2(T_j, T) \approx \left. \frac{\partial f_2}{\partial T_j} \right|_{T_j, T} T_j + \left. \frac{\partial f_2}{\partial T} \right|_{T_{jin}, T_j, T} T \quad (14)$$

$$f_2 = \left(\frac{S}{mc} \frac{\partial U}{\partial T_j} T_j + \frac{US}{mc} - \frac{S}{mc} \frac{\partial U}{\partial T} T \right) T_j - \frac{US}{mc} T \quad (15)$$

The main nonlinearity in the process of heating and cooling the reactor's content is caused by the change of the reactor's jacket temperature T_j . Different temperatures of the reactor's jacket influence the overall heat transfer U , the change of the flow Φ and the heat capacity c_j of the heating–cooling medium in the jacket. The process is fuzzified according to the reactor's jacket temperature T_j , with simple triangular functions. In order to cover the whole operating range we choose ten membership functions ($K = 10$), with maxima at $-25, -21, -18, -9, 4, 27, 37, 49, 70, 94$ and 140 °C. The maxima are chosen so that they best account the nonlinearities of the heat transfer, as shown in Fig. 6.

The rule base of the locally affine fuzzy model for the overall heat transfer U , the flow Φ and the heat capacity c_j of the heating–cooling medium in the jacket in compact form is written in Eq. (14), where T_j is the reactor's jacket temperature. The triangular membership functions ensure that the normalized degrees of fulfilment $\beta_j(T_j)$ are equal to the membership

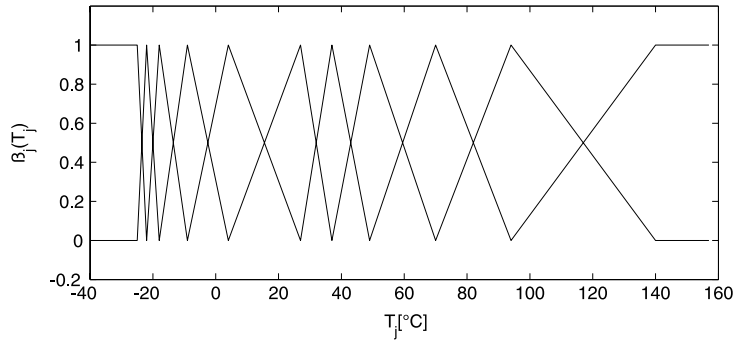


Fig. 6. Membership functions.

values $\mu_j(T_j)$ across the whole operating range for each rule R^j respectively. So the reactor's jacket and core temperature for the next step are calculated via Eq. (16). With the sample time $T_s = 10$ s.

$$\begin{aligned}
 R^j() : & \quad \text{IF } T_j \text{ is } A_1^j \\
 \text{THEN} & \quad U_{\text{fuzzy}}(k) = \beta_{T_j} \Theta_U \text{ AND} \\
 & \quad \Phi_{\text{fuzzy}}(k) = \beta_{T_j} \Theta_\Phi \text{ AND} \\
 & \quad c_{j\text{fuzzy}}(k) = \beta_{T_j} \Theta_{c_j} \text{ AND} \\
 & \quad T_j(k+1) = a_j(k)T_{jin}(k) + b_j(k)T(k) + c_j(k)T_j(k) \text{ AND} \\
 & \quad T(k+1) = a(k)T(k) + b(k)T_j(k) \\
 \text{FOR} & \quad j = 1, \dots, K \\
 \text{WHERE} & \quad
 \end{aligned} \tag{16}$$

$$a_j(k) = T_s \frac{\Phi_{\text{fuzzy}}(k)}{m_j} \tag{17}$$

$$b_j(k) = T_s \frac{SU_{\text{fuzzy}}(k)}{m_j c_{j\text{fuzzy}}(k)} \tag{18}$$

$$c_j(k) = T_s \left(1 - T_s \frac{\Phi_{\text{fuzzy}}(k)}{m_j} - T_s \frac{U_{\text{fuzzy}}(k)S}{m_j c_{j\text{fuzzy}}(k)} \right) \tag{19}$$

$$a(k) = \left(1 - T_s \frac{U_{\text{fuzzy}}(k)S}{mc} \right) \tag{20}$$

$$b(k) = T_s \left(\frac{U_{\text{fuzzy}}(k)S}{mc} \right). \tag{21}$$

The resulting parameters of the locally affine fuzzy model:

$$\begin{aligned}
 \Theta_U &= [235 \quad 312 \quad 353 \quad 445 \quad 541 \quad 567 \quad 602 \quad 644 \quad 680 \quad 722] \\
 \Theta_\Phi &= [3.70 \quad 3.74 \quad 3.79 \quad 3.86 \quad 4.00 \quad 4.06 \quad 4.07 \quad 4.09 \quad 4.11 \quad 4.14] \\
 \Theta_{c_j} &= [3250 \quad 3264 \quad 3289 \quad 3325 \quad 3412 \quad 3443 \quad 3482 \quad 3354 \quad 3622 \quad 3753].
 \end{aligned}$$

6. Validation of the locally affine fuzzy model

For the validation of the locally affine fuzzy model the same input parameters as in the validation of the theoretical model are used, as shown in Table 3. The differences between the theoretical model and the locally affine fuzzy model are minimal. Therefore, no comparison between the simulation results of the theoretical model and the simulation results of the locally affine fuzzy model is shown. To see the difference we calculate the deviation between the simulation of the two models for the reactor's jacket in Fig. 7 and for the reactor's core in Fig. 8.

The difference between the locally affine fuzzy model and the theoretical model is also measured with the root mean square deviation for the reactor's jacket (Eq. (22)) and the reactor's core (Eq. (23)) temperature.

$$\text{RMSD}_j^* = \sqrt{\frac{\sum_{i=1:n} (T_{jin,\text{fuzzy}}(i) - T_{jin,\text{theoretical}}(i))^2}{n}}, \tag{22}$$

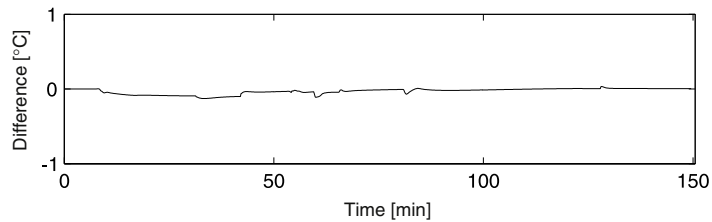


Fig. 7. Deviation between the theoretical and the fuzzy model for the reactor's jacket.

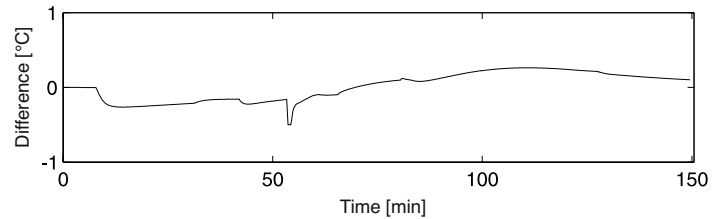


Fig. 8. Deviation between the theoretical and the fuzzy model for the reactor's core.

$$RMSD^* = \frac{\sqrt{\sum_{i=1:n} (T_{\text{fuzzy}}(i) - T_{\text{theoretical}}(i))^2}}{n}, \quad (23)$$

where n is the number of the simulation points.

The deviation for the reactor's jacket is $RMSD_j^* = 0.033$ °C and for the reactor's core is $RMSD^* = 0.165$ °C.

7. Conclusion

On the basis of the physical properties and the measurements taken on the batch reactor for the process of heating and cooling the reactor's core a detailed theoretical model was developed. The main problem with the nonlinearity of the overall heat transfer was successfully solved with the introduction of the correlation equation presented by Petukhov. From the validation results of the theoretical model we can conclude that it successfully describes the behaviour of the real process.

The complexity of the theoretical model for further control development and simulation purposes forced us to build a locally affine fuzzy model on the basis of the theoretical model. The fuzzification of the nonlinear parameters was carried out using the Takagi–Sugeno fuzzy model. The validation of the locally affine fuzzy model shows us that the response of the locally affine fuzzy model is practically identical to the response of the theoretical model. Therefore, the hybrid fuzzy model can be used for control design purposes.

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