

Investigation of Autoclave's Cooling Jacket Static and Dynamic Behaviour

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The dynamical behaviour is necessary in case of investigation of jacketed reactor. In this paper we will show a mathematical model, which is acceptable to determine the removal heat from the chamber function of the time and the volumetric jacket flow as well as define the response of the excited system, which is excited by unit jump function. We will show that in case of increasing jacket flows cause a slow dynamics, and a calculation method of jacket-side heat transfer coefficient based on measuring.

1. Introduction

Nowadays there is increasing demand for energy-rationalization from industrial companies. Our earlier investigation was an autoclave system energy development (specifically energy consumption reducing), where we have inspected the autoclaves cooling jacket static and dynamic behaviour. Part of this task was the jacket side transfer coefficient determination. During our investigation have had possibility for validate the theoretical results in industrial environment.

2. The mathematical model of cooling jacket

The autoclave is a jacketed reactor equipped with a mixer, a cooled / heated jacket, shut-off valves, filling and discharge opening is provided. Several researchers like Bequette (1995), Luyben (1996), Juo (2001), Bihari (2001), Brenner (2006) addressed this process, they usually considered only the static modelling. In our studied autoclave chamber polymerization reaction takes place with heat generation. The homogeneity of the autoclave chamber charge mixer is provided. The removal of heat generated by cooling of the shell chamber. The cooling water flows in a spiral channel with a rectangular cross-section in the jacket. The Figure 1 shows the chamber-jacket heat transfer process.

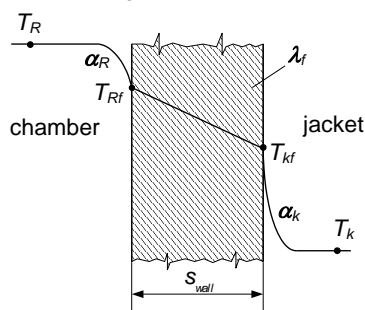


Figure 1: The temperature distribution around the reactor wall

The heat flux between the chamber liquid and the wall – which temperature is T_R – is calculable with Eq. (1), but the α_R must be known:

$$Q_R = \alpha_R \cdot A_h \cdot (T_R - T_{Rf}) \quad (1)$$

The heat energy through in the wall by heat conduction toward the shell-side cooling water, while the temperature decreasing to T_{kf} . The temperature distribution is linear in stationer case, same in Figure 1. In one charge the reaction heat is changed, secondly other difficulties are present, so the non-stationary cases must be taken into account. Inside the wall the temperature distribution calculated by a partial differential equation:

$$c_f \cdot \rho_f \cdot \frac{\partial T_f}{\partial \tau} = \lambda_f \cdot \frac{\partial^2 T_f}{\partial X^2} \quad (2)$$

The heat energy goes through the reactor wall by heat transfer. This heat flux can be calculated by Eq. (3).

$$Q_k = \alpha_k \cdot A_h \cdot (T_{kf} - T_k) \quad (3)$$

The chamber liquid is independent on local, because of the mixing. It would be a perfectly mixed model. On the jacket side the liquid temperature depends on location, it shows on Figure 2.

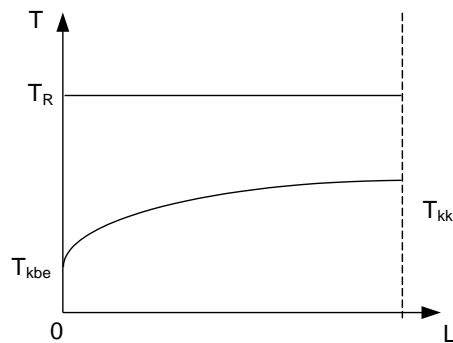


Figure 2: The temperature distribution according to location

The cooling water depends on time and location too in case of a non-stationary operating status, according to the Eq. (4) differential equation.

$$A_{cs} \cdot c_k \cdot \rho_k \cdot \frac{\partial T_k}{\partial \tau} = A_{cs} \cdot v \cdot c_k \cdot \rho_k \cdot \frac{\partial T_k}{\partial X} + \alpha_k \cdot b \cdot (T_{kf} - T_k) \quad (4)$$

where A_{cs} is the $a \times b$ cross-section, L is the length of the flow channel, which is splitted to dx length elemental sized cells.

2.1 Initial conditions of differential equations

The temperature distribution in the wall according to location:

$$T_f(x, \tau = 0) = T_f(x) \quad (5)$$

The temperature distribution in the jacket channels according to location:

$$T_k(x, \tau = 0) = T_k(x) \quad (6)$$

2.2 Boundary conditions of differential equations

The chamber temperature trends according to time:

$$T_R = \Psi(\tau) \quad (7)$$

Changing the temperature and quantity of the cooling water in the jacket channels according to time:

$$T_k = \Phi(x = 0, \tau) \quad (8)$$

$$\dot{V}_k = \Omega(x = 0, \tau) = \text{const.} \quad (9)$$

3. The static and dynamic behaviour of cooling jacket

We investigate the jacketed reactor cooling behaviour, which variable boundary conditioned unsteady state heat transfer simulation calculations are necessary.

The initial condition of this study is the complete heat balance; the polymerization reaction temperature (T_R) equivalent of the autoclave shell and the cooling water temperature. In this complete thermal equilibrium state of the system – in the jacket flows water with 500 m³/h, pump circulated – the feed flow rate is 100 m³/h at 8 °C cooling water at the beginning. In the jacket, the mixed water temperature is will changes effect by the cooling water entering, the temperature decreasing and beginning of the unsteady state heat transfer. Our goal is to determine the wall and the cooling water temperature changes depending on location and time furthermore the changing of the amount of transferred heat depending on time.

In fact, the investigate is define the response of the excited system, which is excited by unit jump function, according to the methods used to control technology. When the responses of the excited functions are stabilized (re-set to the stationary state), another unit jump function will excite the system. This procedure repeats with 100 m³/h steps from 0 to 500 m³/h cooling water range.

We define the amount of the transferred heat from autoclave chamber (Q_R) and the quantity of the transferred heat to the jacket water (Q_k) depends on the time and the location. Changing the quantity of the cooling water (V_k) with jump function, determine the time to set up the new steady-state and the new equilibrium temperature values (Figure 3).

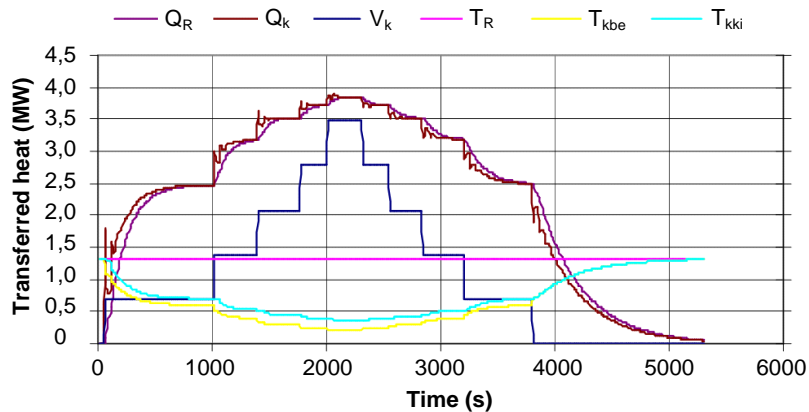


Figure 3: The transferred heat depending of the time

The quantity of transferred heat from the charge is smaller than the expected because some part of this transferred heat is give to cooling of the structural material. This difference will be negligible when approaching a new equilibrium state. This effect is inverted when decreasing cooling water mass flow rate.

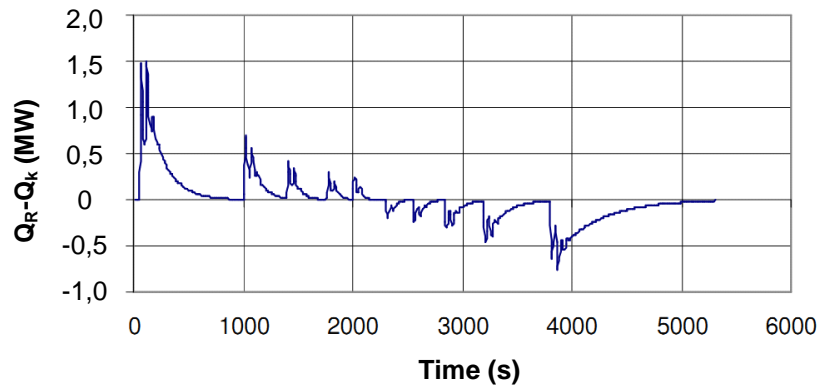


Figure 4: The difference of the amount of the transferred heat from the chamber and the quantity of the transferred heat to the cooling water

4. The heat transfer coefficient determination in the jacket

The heat flux depends on the cooling water quantity thus the heat transfer coefficient also depends on it. In case of the external HTC (heat transfer coefficient, α_k) changing it has an effect on the overall HTC according to Eq. 10.

$$k = \frac{1}{\frac{1}{\alpha_b \cdot \frac{A_b}{A_h}} + \sum_{i=1}^2 \frac{s_i}{\lambda_i \cdot \frac{A_i}{A_h}} + \frac{1}{\alpha_k \cdot \frac{A_k}{A_h}}} \quad (10)$$

Obviously, the internal HTC considered to be constant at the heat transfer process. In the relevant literature there are several equation to determine the jacket HTC. The Reynolds-number can be calculated as a function of the cooling water mass flow. Assuming that the flow pattern will be turbulent in the jacket, the jacket HTC Nusselt number in generally can be determined with the relevant criterial equation. The Eq. 11 shows a general equation for this case.

$$Nu = A \cdot Re^B \cdot Pr^C \cdot \left(\frac{\eta}{\eta_{wall}} \right)^D \quad (11)$$

where Nu Nusselt-number: $Nu = \frac{\alpha_k \cdot d_e}{\lambda}$
 Pr Prandtl-number: $Pr = \frac{c \cdot \eta}{\lambda}$
 A, B, C, D constant.

4.1 Heat transfer coefficient determination with criterial equations

The overall HTC (k) calculation procedure maybe difficult. The main problem that the overall HTC depends on not only the material properties of the flowing fluid but it also depends on the flow pattern, the flow velocity and temperature. In the chemical engineering the generally used procedure that the sought function described with criterial equation based on measuring. Using this method the jacket HTC equation would be described with Eq. 12.

$$Nu = A \cdot Re^B \cdot Pr^C, \quad (12)$$

Where the determinable parameters are: A,B,C.
 These unknown parameters will be calculated the least square method.
 For mathematically, the following extremum problem should be solving:

$$\psi(A,B,C) = \sum_{i=1}^n (Nu_{m,i} - Nu_{c,i})^2 \rightarrow \min, \quad (13)$$

where $Nu_{c,i} = A \cdot Re_i^B \cdot Fr^C$ is the determinable Nu-number, $Nu_{m,i}$ is the measured Nu-number.

The following equation must be solve to determine the A,B,C constants:

$$\frac{\partial \psi(A,B,C)}{\partial A} = 0, \quad \frac{\partial \psi(A,B,C)}{\partial B} = 0, \quad \frac{\partial \psi(A,B,C)}{\partial C} = 0, \quad (14)$$

the conditions: $A,B,C \neq 0, A,B,C > 0$.

The differentials are:

$$\frac{\partial \psi}{\partial A} = 2 \cdot \sum_{i=1}^n (Nu_{m,i} - [A' + B \ln Re_i + C \ln Pr_i]) = 0,$$

$$\frac{\partial \psi}{\partial B} = 2 \cdot \sum_{i=1}^n (Nu_{m,i} - [A' + B \ln Re_i + C \ln Pr_i]) \cdot \ln Re_i = 0,$$

$$\frac{\partial \psi}{\partial C} = 2 \cdot \sum_{i=1}^n (Nu_{m,i} - [A' + B \ln Re_i + C \ln Pr_i]) \cdot \ln Pr_i = 0 \text{ where } A' = \ln A.$$

In vector form the conditions: $g(X) = [-A \quad -B \quad -C]^T < 0$

Formally, this extremum problem with g(x) conditions:

$$\psi(X) \rightarrow \min, \quad g(X) < 0. \quad (15)$$

This penalty-function used for solving:

$$\Phi(X, \sigma) = \psi(X) + \sigma \sum_{y=1}^c \{(\max(g_y(X), 0))\}^2, \quad (16)$$

this procedure is convergent in case of $\sigma_k = 10^{k-1}$.

A Matlab procedure was made to solve Eq. 15, based on the Nelder-Mead method. The given result shown in Eq. 17.

$$Nu = 0,284 \cdot Re^{0,599} \cdot Pr^{0,376} \quad (17)$$

On the Table 1 presented the different between the measured (Nu,m) and the calculated (Nu,c) Nusselt number.

Table 1: Measured and calculated Nusselt-numbers

No.	Re	Nu,m	Nu,c	Error [%]
1	51323	390,36	378,64	3,01
2	102646	592,00	587,15	0,82
3	153969	761,76	758,93	0,38
4	205293	891,41	910,49	-2,14
5	256616	1014,84	1048,60	-3,33
6	307939	1222,29	1176,86	3,72
7	359263	1282,33	1297,47	-1,18
8	410586	1449,59	1411,89	2,60
9	461909	1492,64	1521,17	-1,91
10	513233	1599,56	1626,06	-1,66
11	564556	1747,73	1727,17	1,18
12	615879	1828,94	1824,96	0,22

5. Results and conclusion

We have presented a method to determine the transferred heat incrementation from the rate of differential quotient of transferred heat quantity from the charge according to mass flow variation of the cooling water (see Figure 5). The conclusion is in case of greater amount of cooling water the transferred heat quantity change will decrease; the heat system will lose their dynamics.

We also presented a criterial equation (Eq. 17) to determine the jacket-side Nusselt-number based on theoretical models and industrial measuring results.

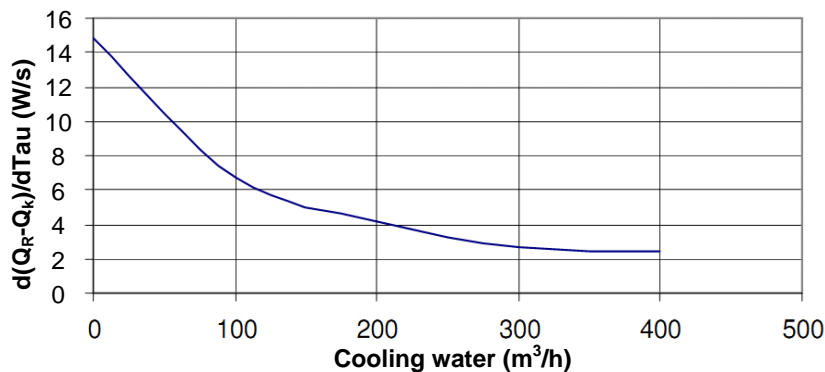


Figure 5: The rate of differential quotient of transferred heat quantity depending of the amount of cooling water

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