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PECULIARITIES IN THE SIZING OF REACTORS WITH STIRRING DEVICES DURING AN EXOTHERMIC REACTION

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Abstract: *The present work aims to address some aspects in the sizing of stirred tank reactors where the exothermic reaction leads to a shortage of heat exchange surface and problems with the utilization of the heat released by the reaction. After computational procedures and applied specific methodologies, a reactor with mechanical stirring, with an irreversible first-order exothermic reaction taking place, has been sized to reach a 70% degree of conversion. In accordance with the specifics of the reaction, a batch reactor with an elliptical bottom and cover and an open turbine agitator with baffles was chosen. Thermal calculations of the reactor have been made to ensure the thermal regime in the presence of a jacket and an external heat exchanger.*

Keywords: *Stirred reactors, Exothermal raction, Dimensioning of reactors, Methods.*

INTRODUCTION

The layout of reactors for homogeneous liquid-phase reactions is mainly stipulated by the nature and properties of the medium, the type of the chemical reaction and the conditions under which it occurs.

The choice of method and device for stirring is determined by the medium viscosity. The stirred reactors designed for carrying out continuous processes in liquid phase differ from he other reactors by the organization of the heat exchange – reactors with jacket, reactor with cooling coil and reactors with external heat exchanger (Froment, G. F., Bischoff, K. B., Wilde J. De., 2011; Luyben, W. L., 2007; Smith, R., 2005).

In jacketed reactors, the cooled or heated area limits the size and shape of the reactor, especially in cases of vigorous exothermal reactions. The reactors with cooling coil do not provide opportunities to create large enough area for cooling or heating. In reactors with external heat exchanger, the heat exchange surface is not a limiting factor for the overall process, allowing slow chemical reactions with high heat effect to occur. In the reactors with stirring or intense mixing, industrial organic or inorganic processe are carried out, e.g. production of potassium persulfate, polymerization of butadiene, reactios of dinitration, sulfonation, nitration and chlorination of hydrocarbons, production of plastics and synthetic rubber, etc. (Harriott, P., 2003; Levenspiel, O., 1999).

In the design and calculation of stirred reactors, they are regarded as aggregates consisting of separate components: vessel, jacket, stirring device. The design of stirred reactors is primarily determined by the type of vessel in which the stirring device is mounted, rather than solely by the construction and type of the stirring device. Therefore, it is important to know the geometrical parameters of the rectors with mechanical stirring (Lecheva-Nedelcheva, A.S., 2012; Paniovska, S., Iliev, V., Mutavchieva, D., 2016; Jakobsen, H. A., 2008).

The aims of the present paper are: dimensioning of a reactor with mechanical stirring by the occurring of exothermal reaction under given operation parameters and available standards, selection of stirring device for the reactor ensuring effective mixing and heat calculations of the reactor to ensure the thermal regime in presence of jacket and external heat exchanger.

EXPOSITION

When exothermal reactions are carried out in batch reactors with mechanical stirring, problems arise with the utilization of the heat released as a result of the reaction and the insufficient heat exchange area.

The object studied is a stirred reactor where 15 000 kg reaction mixture with initial reagent concentration is $C_{A_0} = 0{,}17\ \mathrm{kmol/m^3}$ is supplied and the goal is to reach 70% conversion. An irreversible exothermal reaction of first order takes place in the reactor with heat effect $\Delta H_r = 2{,}8.10^9\ \mathrm{J/kmol}$.

The reaction temperature is $t_r = 120°C$ and the pressure in the reactor is p = 0,3 мPa. The rate constant of the irreversible first-order exothermal reaction is $k_{r_1} = 5{,}5.10^{-5}\ kmol/m^3.s$.

The reaction mixture has the following physical propertis: $\rho_{liq} = 1050\ kg/m^3$; $\mu_{liq} = 0{,}015\ Pa.s$; $c_{p,liq} = 1900\ J/kg.K$; $\lambda_{liq} = 0{,}18\ W/m.K$.

The reaction mixture with initial temperature of $t_{in} = 20°C$ is fed into the reactor for heating through a pump. After completion of the reaction, the reaction mixture is cooled to temperature of $t = 30°C$.

For the purposes of the present study, specific methodologies were developed for reactor dimensioning, choice of stirring device and estimation of the heat regime within the reactor, taking into account the jacket and the external heat exchanger (Jakobsen, H. A., 2008; Domansky, I.V., Isakov, V.P., et al., 1982; Pavlov, K. F., Romankov, P. G., Noskov, A. A., 1990).

The dimensioning of bacth reactors with mechanical stirring is typically involves several stages: determination of the time for completion of the chemical reaction, the time require for one cycle of the reactor, determination of the reaction volume of the reactor and its nominal volume, estimation of the auxiliary operations time and choice of stirring device.

The reactor design is selected according to the required nominal volume and the nature of the reaction. The time for completion of the reaction $t_{ch.r.}$ is a specific parameter that is determined by the characteristic equation of the reactor, reactions' specifics (reversible, irreversible, consecutive, parallel) and the reaction order.

To estimate the total time for one reactor cycle, an assumption is made for the initial total time of the cycle $\tau_{c-initial}$ which is calculated on the basis of the time for completion of the chemical reaction and the provisional efficiency coefficient of the reactor.

The nominal volume of the reactor ϑ_n is calculated using the assumed total cycle time. The calculations necessary for the choice of reactor are shown in Table 1 while the characteristic size and reactor parameters – in Table 2.

Table 1. Results obtained form the calculations necessary for the choice of batch reactor with mechanical stirring.

Parameters	Results
Inirtial reagent concentration A, $C_{A_0}, kmol/m^3$	$C_{A_0} = 0{,}17\ kmol/m^3$
Current reagent concentration A, $C_A, kmol/m^3$	$C_A = 0{,}051\ kmol/m^3$
Time necessary for completion of the first-order chemical reaction, $t_{ch.r.}, s$	$t_{ch.r} = 21\ 890{,}42\ s$
Initially assumed totl cycle time, $\tau_{c-initial}, s$	$\tau_{c-initial} = 3{,}13.10^4\ s$
Set productivity of reactor, $V_s, m^3/twenty\ four\ hours$	$V_s = 1{,}65.10^{-4}\ m^3/s$
Conditional productivity of batch reactor in three-shift operation, $V, m^3/s$	$V = 1{,}41.10^{-4}\ m^3/s$
Nominal volume of the reactor, ϑ_n, m^3	$\vartheta_n = 1{,}96\ m^3$
Reaction volume of the reactor, V_r, m^3	$V_r = 1{,}37\ m^3$

Table 2. Characteristic dimensions and parameters of the selected reactor (Domansky, I.V., Isakov, V.P., et al., 1982).

Technical characteristics of a batch rector with elliptic bottom and lid	
Nominal volume of the reactor	$\vartheta_n = 2{,}00\ m^3$
Reactor diameter	$D = 1{,}4\ m$
Area of reactor jacket	$F_{jacket} = 6{,}5\ m^2$
Surface area of the coil cooler	$F_{coil\ cooler} = 3{,}5\ m^2$
Stirrer diameter	$d_{stirrer} = 50; 65; 80\ mm$
Liquid level height	$H_{liq.} = 1{,}09\ m$ at $\varphi = 0{,}75$ $H_{liq.} = 0{,}77\ m$ at $\varphi = 0{,}5$
Reactor height $H = (1\ \div 1{,}5)D$	$H = 1{,}3.D = 1{,}82\ m$

The selection of the stirring device was based on the reaction mixture characteristics and its viscosity. Initially, the stirrer is selected with respect to the medium's viscosity (in this case $\mu < 10\ Pa.s$) and then the stirrer diameter is calculated through the reactor diameter.

Finally, a check is made to find whether the calculated stirrer diameter corresponds to some standard one. In our case, open turbine stirrer with blades was selected and its characteristic dimensions and parameters are presented in Table 3.

Table 3. Characteristic dimensions and parameters of an open turbine stirrer with blades (Domansky, I.V., Isakov, V.P., et al., 1982).

Parameters and dimensions	Turbine stirrer
Stirrer diameter, $d_{stirrer}, m$	$d_{stirrer} = 0{,}4\ m$
Angular velocity, $\omega, m/s$	$\omega = 3\ m/s$
Rotation speed of the stirrer, $n,\ s^{-1}$	$n = 2{,}83\ s^{-1}$
Blade height, h_b, m	$h_b = 0{,}08\ m$
Blade length, $l,\ m$	$l = 0{,}1\ m$
Distance between reactor bottom and the stirrer, $h,\ m$	$h = 0{,}24\ m$
Distance between reactor wall and the blades, $b,\ m$	$b = 0{,}04\ m$
Coefficient of resistance of the stirrer, ξ	$\xi = 8{,}4$
Mounting height of the stirrer, $h_{mounting},\ m$	$h_{mounting} = 0{,}28\ m$
Shaft diameter, $d_{shaft},\ m$	$d_{shaft} = 0{,}047\ m$
Funnel depth, h_{funnel}, m	$h_{funnel} = 0{,}81\ m$
Power spent to overcome the friction in the seals, N_{seals}, W	$N_{seals} = 17{,}82\ W$
Power to drive the stirrer, $N_{drive\ the\ stirrer}, W$	$N_{drive\ the\ stirrer} = 1855{,}71\ W$
Electric motor power, N_{motor}, W	$N_{motor} = 3000\ W$

After the selection of reactor and stirrer, additional calculation must be made to determine the time for the auxiliary operations including the times for heating the reaction mixture from 20˚C to 120˚C and the time for cooling the reactor from 120˚C to 30˚C (Table 4). The processes of heating and cooling are carried out in reactor jacket.

The selected reactor had nominal volume of $\vartheta_n = 2\ m^3$ and contains $\vartheta_{liq.} = 1{,}5\ m^3$ liquid. The heat exchange surface of the jacket was $F_{jacket} = 6{,}5\ m^2$ which must satisfy the heat balance of the reactor. Therefore, it is necessary to perform heat calculations for the case when the heat exchange process takes place in the jacket, aiming to determine the heat-transfer area of the reactor and compare it with its available surface (Table 5).

Table 4. Results obtained from the additional calculations for determining the time for the auxiliary operations.

Parameters	Results
Time for preparation of the reactor for new cycle, τ_1, s	$\tau_1 = 720\ s$
Time necessary to fill the reactor, τ_2, s	$\tau_2 = 900\ s$
Time necessary to empty the reactor through the orifice, τ_5, s	$\tau_5 = 830\ s$
Time necessary to heat the reaction mixture, τ_3, s	$\tau_3 = 430\ s$
Time necessary to cool the reactor, τ_4, s	$\tau_4 = 4\ 020\ s$
Total auxiliary time, $\tau_{auxiliary}$, s	$\tau_{auxiliary} = 6\ 900 s$
Precised time for one reactor cycle, $\tau_{c-precised}, s$	$\tau_{c-precised} = 2{,}87.10^4\ s$
Initially assumed total cycle time, $\tau_{c-initial}, s$	$\tau_{c-initial} = 3{,}13.10^4\ s$
Reactor mass, $m_{reactor}, kg$	$m_{reactor} = 190\ kg$
Volume of the liquid in the reactor, $\vartheta_{liq.}, m^3$	$\vartheta_{liq.} = 1{,}5\ m^3$

Table 5. Heat calculations of the reactor with mounted jacket.

Parameters	Results
Heat flow through the heat transfer surface of the rector, Q_F, W	$Q_F = 35\ 046{,}5\ W$
Heat flow of the reactor, $Q_{ch.r}, W$	$Q_{ch.r} = 39\ 270\ W$
Heat flow released to the environment, $Q_{environment}$, W	$Q_{environment} = 3\ 930\ W$
Power spent to stir the reaction mixture, N, W	$N = 1\ 670\ W$
Heat losses, $Q_{losses} = 0{,}05.Q_{ch.r}$, W	$Q_{losses} = 1\ 963{,}5\ W$
Nusselt criterion, Nu_1	$Nu_1 = 4\ 420$
Nusselt criterion, Nu_2	$Nu_2 = 1\ 160$
Heat transfer coefficient in stirred medium to reactor wall, $\alpha_1, W/m^2.K$	$\alpha_1 = 1990\ W/m^2.K$
Heat transfer coefficient from reactor wall to the heat carrier, $\alpha_2, W/m^2.K$	$\alpha_2 = 650\ W/m^2.K$
Sum of the thermal resistances, $\sum r_{th.r}, m^2.K/W$	$\sum r_{th.r} = 6{,}6.10^{-4}, m^2.K/W$
Coefficient of heat transfer, K, W/m^2.K	$K = 376\ W/m^2.K$
Temperature difference between the reaction mixture and the heat carrier during the reaction, $\Delta t_{average}$, °C	$\Delta t_{average} = 20$°C
Necessary heat exchange area of the reactor jacket, $F_{necessary}$, m^2	$F_{necessary} = 4{,}66\ m^2$
Available heat exchange area of reactor jacket, $F_{available} = F_{jacket}$, m^2	$F_{available} = F_{jacket} = 6{,}5\ m^2$
Debit of heat carrier necessary to ensure the heat regime in the reactor, $G_{heat\ carrier}$, kg/s	$G_{heat\ carrier} = 0{,}84\ kg/s$

It can be seen from the results presented in Table 5 that the available heat exchange area of the reactor is the heat exchange ares of reactor jacket $F_{нал} = F_p = F_{кожух} = 6{,}5\ m^2$. In this case it is larger than the heat exchange necessary $F_{necessary} = 4{,}66\ m^2$ for the exothermal rection. Therefore, the selected reactor with jacket can realize the heat exchange.

Heat calculations were also made for the case when an external heat exchanger (cooling condenser) is mounted to the reactor. The vapors from the reaction mixture pass in the intertube space with temperature 120˚C, condense and the condensate with temperature 110˚C exits the heat exchanger and flows to the reactor. The cooling condenser selected was a jacketed tubular heat exchanger with jacket diameter D_k = 600 mm; number of tubes n = 161, each with height H = 2 m and diameter of tubes $\emptyset\ 25 \times 2\ mm$.

Table 6. Heat calculations of the reactor with external heat exchanger.

Parameters	Results	
Heat flow carried out by he reaction mixture vapors, Q_{out}, W	$Q_{out} = 9\,170\ W$	
Heat flow for cooling the condensate of the reaction mixture from reaction temperature to the final temperature, $\mathrm{Q_{condensate}}$, W	$Q_{condensate} = 420\ W$	
Total heat flow in the cooling condenser, $\mathrm{Q_{out}} + \mathrm{Q_{condensate}}$, W	$Q_{out} + Q_{condensate} = 9\,590\ W$	
Coefficient of heat transfer of reaction mixture vapors to the surface of the vertical tubes, $\alpha_1, \mathrm{W/m^2.K}$	$\alpha_1 = 337{,}40\ \mathrm{W/m^2.K}$	
Coefficient of heat transfer from the vertical tube wall to the cooling water, $\alpha_2, W/m^2.K$	B1	$\alpha_2 = 4\,890{,}96\ W/m^2.K$
	B2	$\alpha_2 = 1\,572{,}23\ W/m^2.K$
Sum of the thermal resistances, $\sum \mathrm{r_{th.r}}, \mathrm{m^2.K/W}$	$\sum r_{th.r} = 3{,}88.10^{-4}, m^2.K/W$	
Coefficient of heat transfer, К, W/m^2.K	B1	$K = 281\ W/m^2.K$
	B2	$K = 251\ W/m^2K$
Average temperature difference by direct-flow and reverse-flow schemes of fluids flows, $\Delta \mathrm{t_{average}}$, ℃	B1	$\Delta t_{average}^{\rightrightarrows} = 20$℃
	B2	$\Delta t_{average}^{\rightleftarrows} = 44{,}92$℃
Required heat exchange surface area, $\mathrm{F_{necessary}}$, $\mathrm{m^2}$	B1	$F_{necessary} = 17{,}13\ m^2$
	B2	$\mathrm{F_{necessary}} = 0{,}85\ \mathrm{m^2}$
Available heat exchange surface area, $\mathrm{F_{available}}$, $\mathrm{m^2}$	$F_{available} = 23{,}25\ m^2$	
Debit of the cooling water, $G_{\mathrm{H_2O}},\ kg/s$	B1	$G_{\mathrm{H_2O}} = 0{,}23\ kg/s$
	B2	$G_{\mathrm{H_2O}} = 0{,}035\ kg/s$

The calculations were made for two cases. Case 1 (B1): the cooling water flows in the tubular space with initial temperature of 95˚C and final one 105˚C; Case 2 (B2): the cooling water flows in the tubular space with initial temperature of 35˚C and final one 100˚C (Table 6). As can be seen from the results shown in Table 6, the jacketed tubular heat exchanger can condense the reaction mixture vapors at average temperature difference of 20˚C and 44,92˚C. This is possible because the available heat exchanger surface area is larger than the required one.

CONCLUSION

The present paper discusses some aspects of the dimensioning of stirred reactors where the proceeding of an exothermal reaction leads to insufficient heat exchange surface and problems with the utilization of the heat generated by the reaction. A theoretical method for calculation and design of stirred reactors was applied, consisting of individual components: vessel, jacket and stirring device. After carrying out calculation procedures and applying specific methodologies, a reactor with mechanical stirring was dimensioned so it could hold irreversible first-order exothermal reaction aimed to reach 70% degree of conversion. Batch reactor with elliptic bottom, lid and jacket was selected for the realization of the reaction. To ensure effective mixing and achieve the wanted degree of conversion and taking into account reaction specifics, an open turbine stirrer with blades was chosen. It was established that the available surface of the reactor jacket is large enough to utilize the heat generated by the exothermal reaction. The heat exchange process can also be realized in cases when an external jacket-tube heat exchanger of added to the reactor. The specific methodologies for dimensioning of mechanically stirred reactors applied can successfully be used for exothermal reactions of order higher than the first order, too. The theoretical method discussed can also be successfully applied in the education of the students of specialties "Chemical engineering and Chemical technologies".

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