Energetic Efficiency Calculation for a New Experimental Reactor

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The column type reactors play a particularly important role in the chemical industry and technology, because they are successfully used in most of the industrial processes. The inner stirring may be achieved by different mechanical means or by bubbling a gas. This study presents some aspects regarding the heat transfer for a process performed in an experimental bubble gas column reactor. The process in a bubble column reactor was performed at different conditions regarding: temperature, pressure of the inlet gas, nozzle diameters for the inlet gas, packing material inside the reactor; choosing in the end the most convenient conditions for the process energetic consumption efficiency.

Keywords: bubble column type reactor, energetic balance, total heat transfer coefficient

The column type reactors play a particularly important role in the chemical industry and technology, because they are successfully used in most of the industrial transfer processes, such as polymerization, hydrogenation, and oxidation reactions. The inner stirring may be achieved by different mechanical means or by bubbling a gas [1].

The hydrodynamics and its effects on the performance of the columns have been studied in many researches, but the heat transfer characteristics were investigated only by few authors; among them, Cho et al. [2] used a pressurized bubble column in order to determine dynamic characteristics of heat transfer coefficient with viscous liquid medium, analyzing the effects of temperature fluctuations on heat transfer coefficient. Other researchers presented heat transfer analysis in bubble column reactors in different processes. Lin and Fan [3] present heat transfer and bubble characteristics (including bubble size, bubble rise velocity, and bubble formation frequency) from a nozzle in high-pressure bubble columns. Most of the literature on heat transfer in bubble columns focuses on the heat transfer coefficient at the column wall. Heat transfer in shallow bubble columns with internals differs from that in tall bubble columns due to the additional geometric parameters and the effect of the free surface on fluid dynamics. Bubble-on-coil impact, which depends on the horizontal position of the cylinder with respect to the sparger orifices, was proposed by Narayan et al. [4] as a geometric parameter of interest in shallow bubble columns with internals. The effects of coil diameter have been investigated by several authors, although there is disagreement among them [5, 6]. The height of the cylinder is shown herein to affect heat transfer. Tow and Lienhard [7] present the effects and relative importance of these many parameters are investigated with the aim of guiding bubble column dehumidifier design. Deckwer [8-9] published some aspects on mechanism of heat transfer in bubble column reactors. Some authors published computational modeling of hydrodynamics and heat transfer of the processes performed in column reactors, such as Kiran et al. in [10], Krishna R. et al. in [11] and Michele and Hempel in [12].

Heat transfer in column reactors is very important for the process energetic efficiency. Some authors performed their researches in order to develop mathematical correlations for heat transfer coefficient prediction [13] or numerical simulations for the heat transfer in different conditions [14].

Popa et al. [15-18] studied the efficiency of a bubble column reactor in polymerization of methylmetacrylate and copolymerization of it with styrene, varying the conditions of the inlet gas admission – inlet nozzle diameter, different inert gas (nitrogen) pressure, working at different temperatures and using different packing materials.

An esterification process in a bubble column reactor was presented by Stacy et al. [19], but highlighting only the aspects regarding the effect of the reagents on the reaction efficiency. The paper evaluates the performance of an acid-catalyzed bubble column reactor that is highly robust for esterification of free fatty acids to fatty acid alkyl esters; and shows the effects alcohol, feedstock type and quality, alcohol flow rate, and oil feedstock on the reactor performance.

In order to calculate total heat transfer coefficient, the following equations were used:

The general energy balance equation may be written as in equation (1) [20, 21]:

$$Q_1+Q_2+Q_3=Q_4+Q_5+Q_6+Q_7 \qquad (1)$$

where: Q_1 - heat of the raw materials, J; Q_2 - heat needed in the process, J; Q_3 - heat of the chemical reaction, J; Q_4 - heat of the reaction mass, J; Q_5 - heat necessary for heating of the reaction column to the reaction temperature; Q_6 - heat loss, J; Q_7 - heat of the reflux, J.

The energy balance can be also written as in equation (2):

$$q_{del} = q_{tr} = q_{nec} \qquad (2)$$

where: q_{del} - heat delivered by the heating fluid, W; q_{tr} - heat transmitted through the heating area, W, q_{nec} – heat necessary in the process – that is Q_2 in equation (1), W

The transmitted heat can be also written as in equation (3):

$$q_{tr}=KA\Delta t \qquad (3)$$

where: K - total heat transfer coefficient, W/(m^{2}K); Δt - the temperature difference between the heating fluid and the reaction mass, K; A - heat transfer area, m^2.

Heat transfer area can be calculated with the equation (4):

$$A = \pi d_{med}H \qquad (4)$$

where: d_{med} - the average diameter of the column, m; H - the height of the column, m.

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The results of an esterification process performed in a bubble gas column reactor, regarding the calculation of the total heat transfer coefficient, are still inconsistent. Because of that, the authors of the present study proposed a numerical calculation of the total heat transfer coefficient for a discontinuous esterification process performed in a bubble column type reactor. Effects of some process parameters on the energy consumed and on the total heat transfer coefficient were analyzed.

Experimental part

The esterification process was performed in a laboratory glass column reactor provided with heating jacket. The inner stirring was produced by bubbling an inert gas through a nozzle at the bottom of the column. The materials used were 1,2-propylene glycol >99.5% provided by Oltchim S.A. (Romania) and benzoic acid 100% provided by Riedel de Haen AG (Germany)) using the following molar ratio: benzoic acid : 1,2-propylene glycol of 1:2. The catalyst - 0.2% in relation to the raw materials - was *p*-toluenesulfonic acid monohydrate provided by Merck KGaA (Germany).

The experimental column reactor is presented in figure 1.

Fig. 1. Experimental column reactor

The raw materials were introduced into the column, were they have been heated at the reaction temperature, providing samples through a nozzle at the bottom of the column during the reaction process in order to determine the conversion at previously setted times. At the end of the process, the reaction mass was cooled to the ambient temperature.

The experiments were performed using the following conditions: different temperatures (120°C and 138°C); different pressure of the inlet gas (37 Pa, 61.8 Pa, and 123.6 Pa); different nozzle diameters for the inlet gas (0.5mm – 1.3mm); different concentrations of the catalyst (0.5% - 3%); and different packing materials (Raschig rings and beads).

Results and discussions

The paper presents some aspects regarding calculation of the total heat transfer coefficient for an esterification process in a new experimental bubble column type reactor. The process was performed firstly similar to a usual batch reactor [22] at 138°C, but because the temperature was too high and the reaction mass fried at the reactor wall, the process was performed at a lower temperature (120°C), with very good results, taking into account that the reflux was continuous (without it the process cannot occur) during the whole reaction period. The process occurs at similar period of time in the bubble column reactor as in a batch reactor, so there is no need for rising the reaction temperature over 120°C. The experimental determination performed by the authors [22] has shown that this reactor type is more efficient than the conventional batch one.

The esterification process occurs in three steps, regarding the energy balance: the first step (I) is the heating of the raw materials from the ambient temperature to the reaction temperature, the second step (II) is the chemical reaction and the third step (III) is the cooling the reaction mass from the reaction temperature to the ambient temperature.

The results of calculating the heat balance terms and the corresponding thermal challenge ($q=Q/\tau$, W) are presented in table 1.

As it can be seen, the higher thermal challenges appear during the reaction process that is in the second step. Q_{nec} in equation (2) is equal to q_2^{II}, calculated from equation (1).

The total heat transfer coefficient K calculated for the processes performed at 120°C and 138°C respectively are presented in table 2.

From the values of these coefficients it results that the rising temperature over 120°C is not necessary, because the energy consume is bigger and the total heat transfer coefficient K is lower at higher temperature.

In order to determine the optimum amount of the catalyst, the esterification process was performed with different catalyst concentrations. The reaction occurs more rapidly when catalysts concentration grows, but over 2% the growth is not so important as to consume so much of the catalyst.

Using the equations (1) to (4) the results of the heat balance calculations for the esterification process performed at different catalyst concentrations at 120°C are presented in table 3.

Table 1
HEAT BALANCE TERMS

Temp.,°C	Q_2^I, J	Q_2^{II}, J	Q_2^{III}, J	q_2^I, W	q_2^{II}, W	q_2^{III}, W
120	17587.7	212354.2	15133.3	2.44	29.5	2.1
138	20752.7	237086.2	17999.9	1.92	32.93	1.7

Table 2
TOTAL HEAT TRANSFER COEFFICIENT CALCULATED FOR THE PROCESSES PERFORMED AT 120°C AND 138°C RESPECTIVELY

Temperature, °C	K, W/(m^{2}K)
120	590
138	470

Table 3
HEAT BALANCE CALCULATIONS FOR THE ESTERIFICATION PROCESS PERFORMED AT DIFFERENT CATALYST CONCENTRATIONS AT 120°C

Catalyst concentrations, %	Time, h	q_2^{II}, W	K, W/(m^{2}K)
0.5	6,7	8.85	177
1	5,83	10.11	202.2
1.5	5	11.8	236
2	2	29.5	590
2.5	2	29.5	590
3	2	29.5	590

Table 4
HEAT BALANCE CALCULATIONS FOR THE ESTERIFICATION PROCESS PERFORMED AT DIFFERENT PRESSURES OF THE INLET GAS

Pressure, Pa	Time, h	q_2^{II}, W	K, W/(m^2K)
37	2,8	20.82	416.4
61.8	2,5	23.59	471.8
123.6	2	27.22	544.4

Table 5
HEAT BALANCE CALCULATIONS FOR THE ESTERIFICATION PROCESS PERFORMED AT DIFFERENT INLET NOZZLE DIAMETERS

Nozzle diameter, mm	Time, h	q_2^{II}, W	K, W/(m^2K)
0.5	2.2	27.22	544.4
0.6	2.1	29.5	590
0.7	2	29.5	590
0.8	2	29.5	590
0.9	2	29.5	590
1.1	2	29.5	590
1.2	2	29.5	590

Table 6
HEAT BALANCE CALCULATIONS FOR THE ESTERIFICATION PROCESS PERFORMED WHEN PACKING MATERIALS HAVE BEEN USED

Packing material	Time, h	q_2^{II}, W	K, W/(m^2K)
No packing	2	29.5	590
Rashig rings	2	29.5	590
Beads	2	29.5	590

Table 7
KINETICS CALCULATION OF THE PROCESS PERFORMED AT DIFFERENT TEMPERATURES

Temperature, °C	Kinetics calculation	R^2
120	$y=0.001x^2-0.989x+150.3$	0.958
138	$y = 0.003x^2-1.554x+171.2$	0.959

Table 8
KINETICS CALCULATION OF THE PROCESS PERFORMED AT DIFFERENT PRESSURES OF THE INLET GAS

Pressure, Pa	Kinetics calculation	R^2
37	$y = 0.011x^2-2.737x+197.9$	0.988
61.8	$y = 0.009x^2-2.478x+199.3$	0.987
123.6	$y = 0.011x^2-2.751x+193.4$	0.993

Table 9
KINETICS CALCULATION OF THE PROCESS PERFORMED AT DIFFERENT CATALYST CONCENTRATIONS

Catalyst concentrations, %	Kinetics calculation	R^2
0.5	$y = 0.001x^2-045.9x+211.4$	0.986
1	$y = 0.003x^2-1.509x+211.5$	0.970
1.5	$y = 0.003x^2-1.488x+191.1$	0.879
2	$y = 0.013x^2-3.385x+247.6$	0.958
2.5	$y = 0.013x^2-3.359x+243.4$	0.936
3	$y = 0.012x^2-3.341x+248.6$	0.966

Table 10
KINETICS CALCULATION OF THE PROCESS PERFORMED USING DIFFERENT PACKING MATERIALS

Packing material	Kinetics calculation	R^2
No packing	$y = 0.013x^2-2.891x+194.9$	0.993
Rashig rings	$y = 0.009x^2-2.318x+181.8$	0.977
Beads	$y = 0.010x^2-2.496x+177.6$	0.934

It can be observed that using the catalyst concentration of 2% is the best way of performing the esterification process in the bubble column reactor, because the total heat transfer coefficient K rises no more after using higher catalyst concentration.

Using the equations (1) to (4) the results of the heat balance calculations and the corresponding thermal challenge ($q=Q/\tau$, W) for the esterification process performed at different pressures of the inlet gas are presented in table 4.

It can be observed that using the pressure of the inlet gas of 123.6 Pa the reaction period is shorter and the total heat transfer coefficient K has the maximum value.

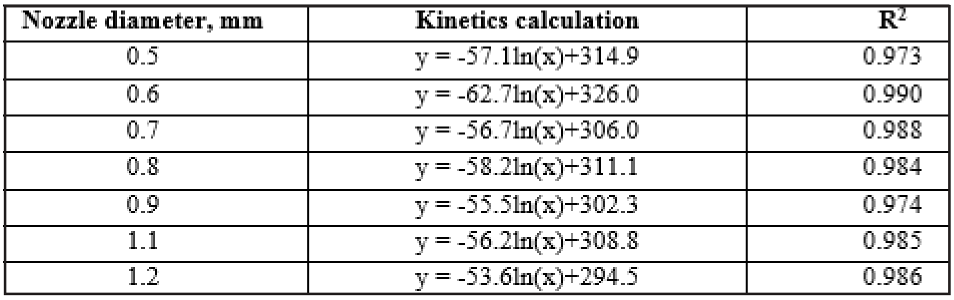
Similar calculations can be made for the other conditions in which the esterification was performed with and without packing material. The results are presented in table 5 - for the esterification process performed at different inlet nozzle diameters; and in table 6 - when packing materials have been used inside the column.

It can be seen that when using different inlet nozzle diameters, the performance of the column is not influenced after increasing the diameter over 0.6mm, so this nozzle diameter was used in the following experiments.

The use of packing material inside the column is not necessary for this process, regarding the energy efficiency,

Table 11

KINETICS CALCULATION OF THE PROCESS PERFORMED USING DIFFERENT DIAMETERS OF THE INLET NOZZLE



Nozzle diameter, mm	Kinetics calculation	R^2
0.5	y = -57.1ln(x)+314.9	0.973
0.6	y = -62.7ln(x)+326.0	0.990
0.7	y = -56.7ln(x)+306.0	0.988
0.8	y = -58.2ln(x)+311.1	0.984
0.9	y = -55.5ln(x)+302.3	0.974
1.1	y = -56.2ln(x)+308.8	0.985
1.2	y = -53.6ln(x)+294.5	0.986

because the value of the total heat transfer coefficient K is the same in all cases.

Kinetics calculation for an esterification process represents, as it is known, the variation of the acid number on time.

The results of the kinetics calculation of the process presented above performed in different conditions are presented in table 7 to 11, where *y* is the value of the acid number [ml KOH/g], and x is time [min].

Conclusions

The esterification process in a bubble column reactor was performed at a usual batch reactor temperature of 138°C, and then at a lower temperature (120°C), with very good results regarding the total heat transfer coefficient K and the energy consumption.

The process was performed, as well, at different catalyst concentration, choosing the most convenient concentration of it (2%) for the process efficiency.

When the esterification process was performed at different pressures of the inlet gas, using the pressure of the inlet gas of 123.6 Pa the reaction period is shorter and the total heat transfer coefficient K has the maximum value.

When using different inlet nozzle diameters, the performance of the column is not influenced after increasing the diameter over 0.6mm.

The use of packing material inside the column is not necessary for this process, regarding the energy efficiency, because the value of the total heat transfer coefficient K is the same in all cases.

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Manuscript received: 15.06.2015