A SIMULATION STUDY OF HEAT TRANSFER IN POLYMERIZATION REACTORS

by

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In this paper, the heat transfer in polymer reactors has been investigated. The study of various methods of heat transfer in jacketed agitated vessels and the impact of altering different agitators on the heat transfer are indicated. A computer program is developed to calculate the heat transfer parameters and the heat duty required for each case. The PVC polymer reactor in the Egyptian Petrochemical Company is chosen as a case study. This reactor is modeled by Microsoft Excel and simulated by a VISIMIX simulation program version turbulent SV. In addition, the chemical reaction is modeled by Aspen HYSYS V8, and eventually the modeling results are validated with the actual design data. Meanwhile, a comparison between various heat transfer methods is generated to set the preferable design and the topmost impeller for high heat transfer conditions. Furthermore, this preferable design is adopted to analyze the alteration on its performance. The result indicates that, the retreating turbine impeller is the best for a high inside heat transfer coefficient and the half coil jacket is the best for a maximum outside heat transfer coefficient. The performance investigation shows that this design is preferable for the optimum recommended flow velocity in the jacket of v = 2.3 m/s, as the outside heat transfer coefficient would increase by 31.47%. Finally, the new approach which is released by Vinnolit Uhde Company is applied and its result show that the heat duty would increase by 32% due to the installation of an inner cooler inside the reactor wall, which represents a significant stride for a high performance polymer reactor.

Key words: *heat transfer, polymer reactor, performance, new approach*

Introduction

The prevalent term for a type of jacketed agitated vessels which are used excessively in petrochemical industry is the *Batch Reactor* [1]. This kind of reactors is utilized for an assortment of processes, such as chemical reactions, batch distillation, and polymerization, which requires a precise control of two important issues, primarily mixing to accomplish a homogeneous batch and secondly the heat of the reaction to hold the batch at the desired temperature. The batch reactor is equipped with an agitator for the sake of an appropriate mixing process. The selection of an agitator is obviously critical since it directly impacts the whole operation and especially the batch heat transfer coefficient, the pattern of agitation and the duty required. In general, the agitators [2] can be classified into three types, according to the pat-

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tern of the flow generated, including radial, axial and hydrofoil impellers. On the other hand, this reactor is designed with a jacket for adequate heat transfer in the form of an external jacket or internal coils for adding or removing heat. As a matter of fact, there are three types of external jackets in the industry, namely: half coil jacket, dimple jacket, and conventional jacket. Each type has its specific design, guidelines, and empirical equations, while each sort ought to be opted for according to the criteria of the process. The intensity of the heat transfers depends on three main factors, including the operating parameters, the design parameters, and the medium's thermal properties.

Many contributions have been made for studying the alteration of the design of the jacketed agitated vessel and evaluating the heat transfer coefficients. In these studies, valuable experimental and analytical data have been revealed for setting the equations of heat transfer. Luyben [3] provided an overview of the sorts of chemical reactors and demonstrated the heat transfer methods. The research book by Kars and Hiltunen [4] set an extended view of the purpose of agitation in the industry and discussed the designs and the conceivable arrangements of agitators. Hewitt *et al.* [5] focused his attention on clarifying the types of coils and studied each type's configuration and benefits. Then, the author supported his study with a brief to increase the heat transfer inside the coil through applying Jeschke [6] empirical correlations. For an appraisal of jacket design, Carpenter [7] and Sharratt [8] concentrated on setting the guidelines that must be considered in the design of jackets and coils, especially the minimum flow velocity which ought to be v = 1-1.5 m/s for a plain jacket, 2.3 m/s for a half-pipe jacket, 0.6 m/s for a dimpled jacket and 1.5 m/s for an internal coil. One of the focal researches in the heat transfer of agitated vessels is the study by Dream *et al.* [9] that identified the distinctive sorts of the jacketed vessels and conducted the set of correlations for both inside and outside heat transfer coefficients, according to the type of the agitator and the design of jacket respectively. Da Silva and De Moraes [10] presented a summary of the literature concerning heat transfer surfaces in agitated vessels equipped with jackets, helical coils, spiral coils or vertical tube baffles. Moreover, they carried out the parameters' effect on Nusselt equation for these surfaces. The concept of enhancing the performance of heat transfer in reactors has been recently developed in the research by El-Shazly and Elsayed [11]. In this study, two pumps were inserted in the system to overcome the fouling effect. The result indicated that the heat transfer coefficient increased by 21%. Ozdemir and Durmaz [12] suggested a new Nusselt function for the heat transfer mechanism of agitated vessels. Results showed that the heat transfer coefficient had a constant value under non-agitated conditions and increased depending on agitation intensity, furthermore it decreases when the sucrose concentration increases.

The scope of work

The objective of the present investigation is to provide an intensive view of the various methods of heat transfer and the sorts of agitators used in polymer reactors. The scope of this study is aimed at comparing between each heat transfer method with respect to the change in the agitator type in order to select the topmost design and show the influence of altering performance on design factors, such as flow velocity, pressure drop, nominal pipe diameter, angle of half coil, and inlet temperature for this selected design. Unlike the previous studies, this paper presents a new approach to a completely new reactor design improved by Vinnolit Uhde Company for enhancing heat transfer in a superb way.

Methodology

This study commences by studying the types of jackets, investigating the sorts of agitators and recognizing all the parameters which affect the heat duty required for a polymerization reaction, especially the changeable parameters. After that, the governing equations of the heat transfer for both batch side and jacket side will be set for the modeling program to evaluate the heat transfer behavior for each case. Then, a polymer reactor in the Egyptian Petrochemical Company is chosen to numerically compare between each design and select the most preferable one to analyze its performance. Finally, a new approach is applied to study the progression on the heat transfer.

Modelling

To assess the performance of a cooling system while altering different types of both jackets and impellers for obtaining an efficient heat transfer condition, a logical program should be used. The first step, in the present work, is establishing a modelling program by Microsoft Excel to utilize a tool that can calculate the behaviour of heat transfer. This program is designed according to the database of Visual Basic within Microsoft Office [13] to define the physical properties of fluids and the design parameters. The solution sequence flow diagram of the program is built as shown in fig. 1.

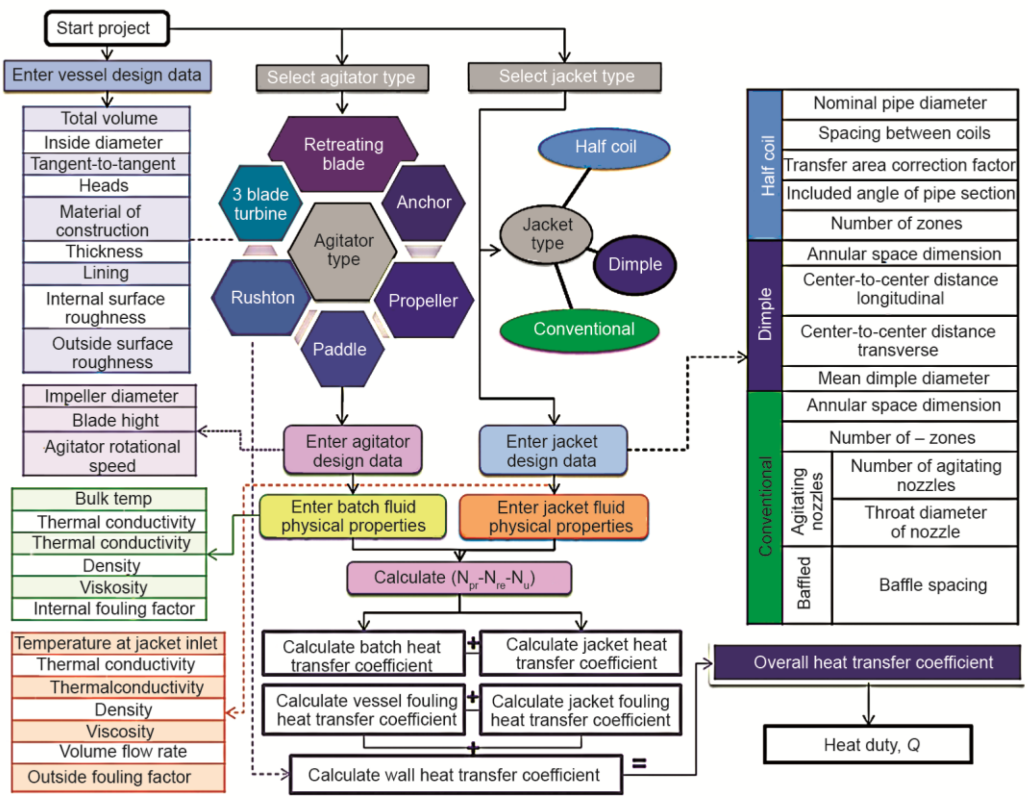

Figure 1. Flow diagram of modeling program

Mathematical modeling of the governing equations

The rate of heat transfer to or from a batch fluid in a reactor is a function of the physical properties of the batch fluid and the jacket medium, the vessel geometry and the type of the agitator. The overall heat transfer coefficient in a jacketed agitated vessel system can be determined from the energy balance equation and the empirical correlations for each design. The following assumptions are introduced to describe the simple form of an overall heat transfer coefficient, which are: the flow is turbulent and in a steady-state, the thermal properties of the batch and the jacket fluid are constant, the energy balance equation is composed of a series of resistances, the heat transfer from jacket wall to batch fluid is a convective heat transfer, and the heat transfer through the vessel wall is based on conduction through the vessel material of thickness, X, with a material thermal conductivity of, κ. The total resistance can be defined by the total overall heat transfer coefficient which is given by eq. (1):

$$\frac{1}{U}=\frac{1}{h_\mathrm{b}}+\frac{1}{h_\mathrm{j}}+\frac{1}{h_\mathrm{w}}+F_\mathrm{b}+F_\mathrm{j} \tag{1}$$

The governing empirical equations of batch heat transfer coefficient, h_b, through different agitators were indicated by Dream [9]. In the same way, the governing empirical equations of jacket heat transfer coefficient, h_j, through various heat transfer methods were indicated by McKetta [14] and Garvin [15]. The heat duty is the gain value which evaluates the capability of cooling or heating system to remove or add heat to the overall process. This can be determined by eq. (2):

$$Q=UA\Delta T_\mathrm{mean}=mC_p\Delta T \tag{2}$$

The heat of polymerization can be determined by the general equation of reaction eq. (3):

$$q_\mathrm{r}=\dot{m}H_\mathrm{p}\frac{\zeta}{t} \tag{3}$$

Case study

Polyvinyl chloride PVC is one of the most widely spread polymers. The PVC polymer reactor in the Egyptian Petrochemical Company which is located in Alexandria-Egypt was chosen to be the case study. The polymerization process of PVC can be divided into three continuous processing plants. Chlorine is the basic raw material which is produced after the chemical reaction with salt and water. Then, the VCM is obtained from ethylene and acetic acid in the presence of an appropriate catalyst with chlorine. Finally, the VCM is polymerized into PVC in batch reactors, and then dried, as shown in the process flow diagram in fig. 2 for the PVC plant.

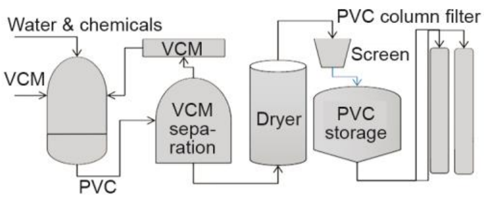

Figure 2. The PVC process flow

The PVC plant of the Egyptian Petrochemical Company has four reactors, each reactor has V_v =70 m^3 capacities. The exothermic heat of the reaction is removed by passing Φ = 200 m^3 per hour cooling water at 26 °C through the jacket and 90 m^3 per hour chilled water at 10 °C through four baffles. The temperature of the reaction should be held at 56 °C. The design of the cooling jacket is half coil, 4" diameter, schedule 40 and its material is carbon steel. The VCM is charged to the reactor with the amount of M = 24.2 kg, and then the demineralized water is charged to the reactor with chemicals as an emulsifier. The design of one reactor is shown in fig. 3.

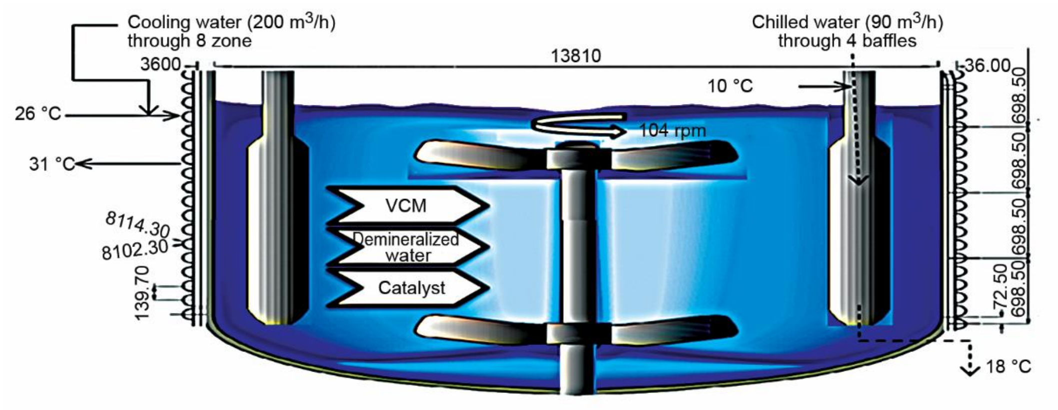

Figure 3. Polymer reactor design

Finally, the VCM monomer is transformed into PVC in 5-6 hours, according to the specification of the PVC grade required, as shown in the simulation by Aspen HYSYS in fig. 4.

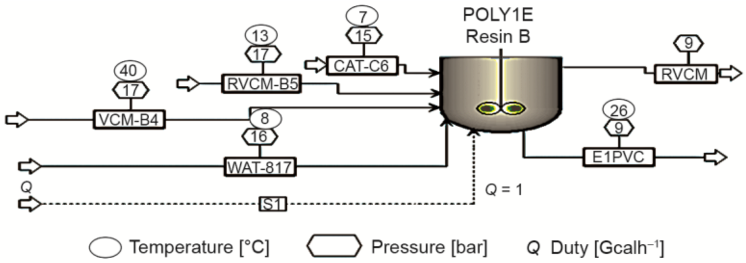

Figure 4. Process simulation

The heat of the reaction which should be removed through one batch is approximately 3.2691e+10 joule. This heat is based on the VCM polymerization energy H_p = –97.6 kJ/mole, according to Saeki and Emura [16]. Subsequently, the heat of the reaction and the heat duty of the cooling jacket should be balanced. However, in operating conditions with the alteration of changeable parameters, this balance would not be achieved.

Code validation

In order to check the validity of the modeling program which is used in this study, it is validated by comparing its results with the actual design data of the PVC polymer reactor which was documented in the mechanical data book for the PVC plant, volume X.IV. The comparison shows a convenient agreement between results, as shown in tab. 1.

New approach

A new approach has been released by Vinnolit Uhde Company which is one of Europe's leading PVC producers. The company has upgraded the design of the entire PVC plant. Through this way, it released a new approach of cooling the polymer reactors by installing an inner cooler inside the reactor wall, as shown in fig. 5. Therefore, to apply this approach

Table 1. Comparison between the present work actual data

Comparison factor	Present work	Actual design	Units	Percentage deviation
Overall heat transfer coefficient	702	U_{mean} = 693	[$Wm^{-2}°C^{-1}$]	1.2%
Heat duty of jacket	1080	1052	[kW]	2.6%
Heat of polymerization	1482	1514	[kW]	2.11%

Figure 5. Design of new approach

to the case study, the value of the batch heat transfer coefficient for the same selected impeller will be changed due to the new correlation of Nusselt number.

This new correlation of Nusselt number was developed by Bondy [17]:

$$N_U = 1.4 N_{Re}^{0.65} N_{Pr}^{0.33} \left(\frac{\mu_b}{\mu_{b,w}} \right)^{0.14} \tag{4}$$

The heat transfer coefficient for the batch side can be calculated:

$$h_b = N_U^* \frac{\kappa_b}{D_v} \tag{5}$$

The correlation by Garvin [18] of the inner cooler heat transfer coefficient is set:

$$h_j = 0.0225 N_{Re}^{0.795} N_{Pr}^{0.495} \exp[-0.025 \ln(N_{Pr})^2] \left\{ 1 + 0.059 \left[N_{Re}^* \left(\frac{D_e}{D_v} \right)^2 \right] \right\} \frac{\kappa_j}{D_e} \frac{D_{ci}}{D_{co}} \tag{6}$$

Consequently, these equations were inserted into the program, as done before for other types of jackets, to calculate the heat transfer coefficient and the heat duty.

Result and discussion

The result data indicated by the program has been divided into four sectors.

Agitators comparison

The result of altering different agitators indicated that the impeller type will have quite an effect on the batch heat transfer coefficient. In practice, the agitator that can resist fouling on heat transfer surfaces will be beneficial. In view of the preferable heat transfer conditions, the comparison between different agitators is indicated as shown in fig. 6.

The highest local heat transfer condition occurs with the retreat curve impeller, and the second most approximate one is Rushton impeller. That is due to the high value of multiplicity factor for the retreat curve impeller which is equal to 0.68 and for Rushton impeller which is equal to 0.74 when the other factors in the impeller equation are kept constant. The heat transfer coefficient of the batch side is more than the jacket one due to the effect of the large impeller diameter and its high speed that would lead to the high value of Reynolds number reaching 5.807 E+7.

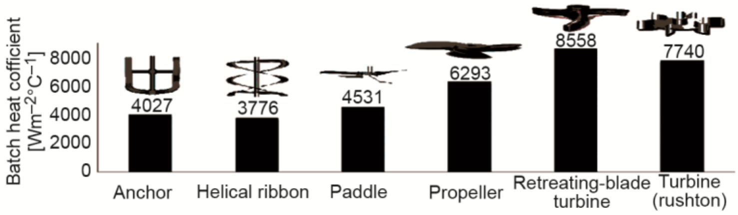

Figure 6. Comparison between different agitators

Comparison between heat transfer methods and half coil jacket

The comparisons between heat transfer methods depend on altering each method at the same operating conditions, such as the volume flow rate, as well as the same design factors, such as the nominal jacket diameter.

Dimple jackets vs. half coil

The comparison result data of the dimple jacket *vs.* the result of the half coil is indicated as shown in fig. 7. When the mean dimple diameter of a dimple jacket is equal to the half coil nominal diameter, the dimple center-to-center distance longitudinal and transverse are equal to the center-to-center distances between the coils.

The matching design of the dimple jacket to the half coil jacket proved that this design is not acceptable. Because the dimple jacket has a higher pressure drop than that of the half coil by 260% due to its high flow velocity, which is beyond the recommended minimum. This enormous value of pressure drop [15] is because the dimples of the jacket cause an enormous turbulence. While this turbulence is minimal by reducing the velocity to the recommended value of v = 0.6 m/s, the heat duty would be reduced by 57% at 456 kW within the normal pressure drop at 36 kPa. Therefore, this design is not convenient as well.

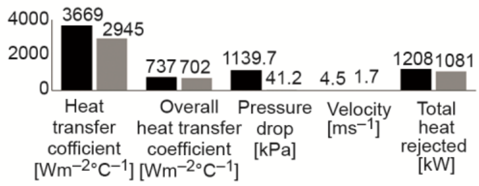

Figure 7. Comparison between dimple jacket *vs.* half coil

Conventional jackets vs. half coil

The most suitable interior-matching design is that of the simple conventional jacket due to its minimal heat transfer coefficient value of h_j = 92 W/m^2°C when its annular space dimension is equal to the inner diameter of the half coil jacket. On the other hand, when the baffles are added to the conventional type, the result is indicated as shown in fig. 8.

Because there are no internal segments that can cause any turbulence in the simple conventional type and the flow velocity is almost zero, this type is no longer used. While the baffles are added at the recommended flow velocity of v = 1.5 m/s with the baffle spacing of 0.07 m, it is shown that this type is the most approximately valid design, because its heat duty decreases a little by 10% than that of the half coil. However, while the pressure drop in the baffled type is higher than that of the half coil by 77%, the heat transfer coefficient of the baffled type is less than that of the half coil jacket by 48%. That is traced back to the inferior distribution of heat transfer fluid due to the clearance [19] that must be permitted between the baffles and the inside of the jacket. Consequently, the actual velocity may be a fraction of the calculated value. Eventually, this design may be applicable, but it is hard to achieve the same half coil heat duty because it requires 0.0245 m baffle spacing with the exact flow velocity v = 4.4 m/s, which is beyond the recommended value. On the other hand, when two agitating nozzles per zone size 3 inch at 0.0285 m throat diameter are added to the simple conventional jacket to match the half coil with the specified recommended flow velocity v = 5 m/s, the result is set as shown in fig. 9.

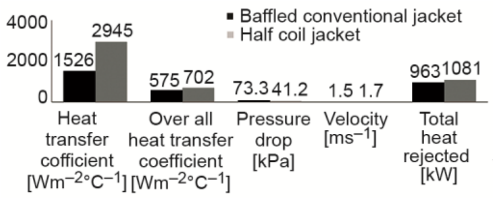

Figure 8. Comparison between conventional baffled jackets *vs.* half coil

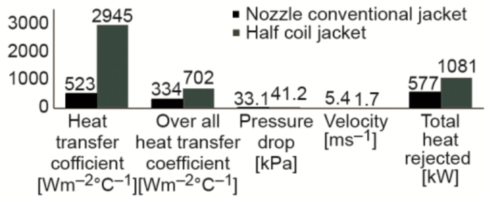

Figure 9. Comparison between agitating nozzles conventional jacket *vs.* half coil

The result shows that the agitating conventional jacket is not applicable due to its inferior heat transfer conditions. The heat duty decreased by 46% and the heat transfer coefficient decreased by 82%. That is traced back to the fact that these nozzles [14] produced a localized turbulence with the spiral flow tangentially to the jacket wall, this local turbulence had an effect on the overall heat transfer.

Comparison between heat transfer methods summary

The comparison result summary between the types of jackets is indicated as shown in fig. 10.

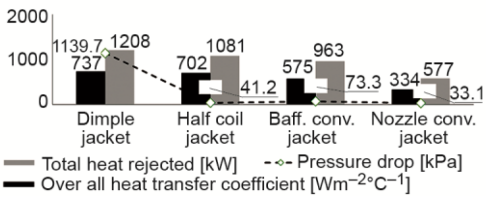

Figure 10. Comparison summary between heat transfer methods

The last figure illustrates that the design that should obviously be selected is the half coil jacket since its heat duty is the maximum with respect to the minimum pressure drop. Furthermore, the value of the flow velocity and the pressure drop is convenient. The wall resistance is moderate due to the sufficient thermal conductivity of carbon steel. Finally, the overall heat transfer coefficient seems advisable as the typical range for a well-designed half coil jacket that should be h_j = 400-700 W/m^{2}K as set by Carpenter [7].

Performance results and discussion of the selected design

The study of the performance of the selected design depends on analyzing one factor when the other factors are kept fixed to study the impact of any alterations in this factor.

Flow velocity in the jacket

The result of alter velocity versus the change in pressure drop is indicated as shown in fig. 11.

The result illustrated that at the maximum limit of velocity v = 3 m/s, the pressure drop increases to the upper limit at 144 kPa. The operating flow velocity v = 1.7 m/s in the half coil jacket is beyond the minimum recommended by Sharratt [8] which should be v = 2.3 m/s. The last figure emphasizes that the flow velocity should be at least v = 2.1. Therefore, the effect of altering different velocities on the heat transfer coefficients is indicated as shown in fig. 12.

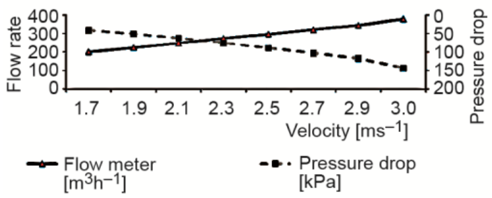

Figure 11. Flow velocity in jacket performance

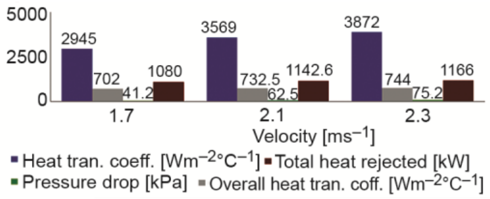

Figure 12. Comparison between recommended and actual velocity

The figure showed that at the recommended velocity v = 2.3 m/s, the pressure drop slightly increased to a normal value at 75.2 kPa and the heat transfer coefficient increased by 31.47%. In addition, the heat duty partially increased by 8%, which represents a valuable progress in heat duty. That is traced back to the dramatic rise in Reynolds number from 122163 to 166103.

Nominal diameter

The result of altering different nominal diameters is indicated as shown in fig. 13.

The result demonstrates that the nominal diameter 0.1 m represents an appropriate selection which achieves a convenient pressure drop at 41 kPa. On the other hand, at 0.075 m nominal diameter, the flow velocity increases to v = 2.9 m/s and the pressure drop increases to a high value at 205 kPa. Therefore, this case is not acceptable due to its minimal cross section area, which causes immense turbulence. In the view of heat transfer, the comparison is shown in fig. 14.

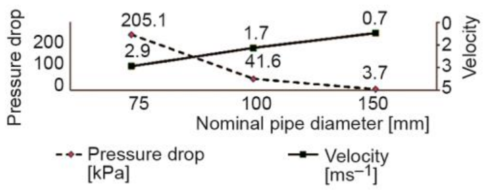

Figure 13. Nominal diameter performance on pressure drop

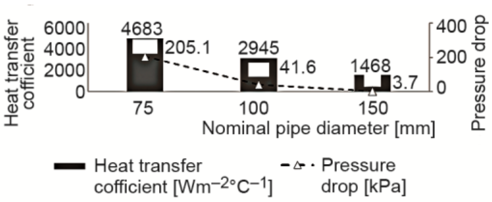

Figure 14. Nominal diameter performance on heat transfer

In the same way, at nominal diameter 0.15 m, the flow velocity is reduced to v = 0.7 m/s, and the pressure drop is reduced to 3.7 kPa. Although the pressure drop seems convenient, the heat transfer coefficient is reduced by 50%.

Angel of half coil

The result of changing the angle of the half coil is illustrated as shown in fig. 15.

The appropriate angle should be 180° which achieves a convenient pressure drop. On the other hand, at 120°, the flow velocity increases to v = 4.3 m/s, which is out of the scope of the recommended flow velocity and pressure drop.

Inlet temperature

The result indicates that the inlet jacket temperature is a very critical parameter. That is due to the fact that any slight increase in it causes a dramatic reduction in heat duty. The heat duty would be decreased by 12.6% if there is a rise of four degrees above normal, as shown in fig. 16.

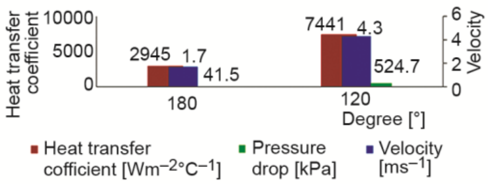

Figure 15. Angle of half coil performance

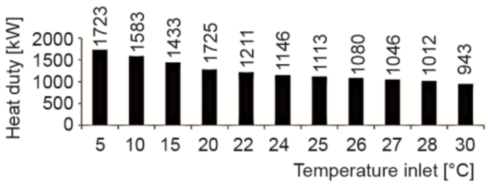

Figure 16. Inlet temperatures performance

The figure shows that the normal range of the inlet temperature is 25-28 °C to achieve a convenient heat duty. Moreover, the critical value of inlet temperature is 30 °C. The alteration in inlet temperature could be traced back to many factors, such as environmental and feed water conditions.

Fouling factor

The result suggests that the fouling factor is an important factor, as shown in fig. 17.

The normal operating fouling factor on the jacket side should be $F_j = 0.00011$ m^2°C/W, while the maximum serious value is 0.00042 m^2°C/W. According to TEMA, the normal range of a fouling factor for cooling tower feed water is $F_j = 0.0001$ – –0.00035 m^2°C/W.

Comparison between half coil jacket and new approach

The comparison result between the new approach and the half coil is set as shown in fig. 18.

The previous result showed the enormous benefits of the new approach, especially on heat duty which is increased by 32%. However, the heat transfer coefficient of the jacket side slightly decreased by 10% and the heat transfer coefficient of the batch size decreased by 15%, but the overall heat transfer coefficient is increased by 38%. That is traced back to the fact that, firstly the wall heat transfer coefficient is increased by 119%, $h_w = 1184$-2599 W/m^2°C due to the reduction of heat transfer thickness from 0.038 m of the reactor wall thickness to 0.006 m of the pipe thickness. A second reason is the high turbulence which was revealed at the outside corrugated tube wall. Eventually, a high differential temperature is

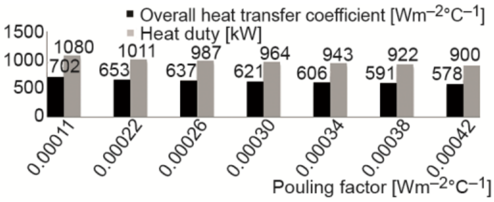

Figure 17. Comparison between different fouling factors

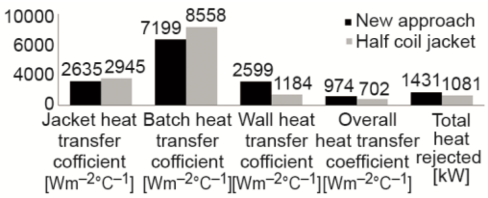

Figure 18. Comparison result between the new approach and the external half coils

produced between the reactor medium and the water in the jacket, owing to the new correlations of Nusselt number with the same Reynolds number. The new approach features are:

– A temperature difference increase of 56%, the heat duty of the new inner jacket fulfills the requirements and overcomes the heat of the reaction by 95%, instead of 67%.
– The new inner jacket reduces the usage of chilled water in the buffer by 59% to be 290 kW, instead of 720 kW, therefore the number of buffers inside the reactor will be reduced to two buffers, as shown in fig. 2, for the new design by Vinnolit Uhde Company.
– A minimal reaction time to be cooled by rate α = 1.07 °C per minute, instead of 0.8 °C per minute, therefore the cooling rate is increased by 33%.

Conclusion

The aim of this paper is to investigate the criteria for heat transfer in a polymer reactor. A case study is adopted to ensure, numerically, the difference between the types of jackets and agitators as well the ability to enhance heat transfer conditions. According to the previous analyses, some general conclusions could be noted to ensure an appropriate selection of jackets.

- The conventional jacket is often used in a small vessel design up to 3.4 bar when the recommended flow velocity is v = 1.5 m/s.
- The dimple jacket has better heat transfer characteristics due to the high turbulence generated by the dimples, but the pressure drop limits the flow velocity to v = 0.6 m/s.
- The half coil has sufficient heat transfer characteristics due to high velocity, turbulence and the fact that it can be divided into multi-pass zones when the recommended flow velocity is v = 2.3 m/s.

The guidelines for the case study:

- The maximum value of the inside heat transfer coefficient depends on the selection of the retreating turbine blade and secondly the Rushton impeller.
- The maximum value of the outside heat transfer coefficient depends on the selection of: firstly the half coil jacket, and secondly the baffled conventional jacket.
- The operating flow velocity in the jacket is beyond the recommended, at which the outside heat transfer coefficient would increase by 31.47%.
- The appropriate value of the nominal diameter of the half coil is 4 inch with 180° angle, the critical inlet temperature in the jacket is 30 °C, and the maximum limit of fouling factor is F_j = 0.00042 m^2°C/W.
- The heat duty would increase by 32% by applying the new approach.

Finally, the heat transfer in a polymer reactor is crucial to control the outcome of a process at the desired temperature. Thus, a struggle is created to distinguish between various types of heat transfer methods to select the most convenient design for each case through the analyses of its performance. The design factors have an evident influence on the overall process which should be surveyed quite thoroughly using suitable modeling and simulation programs in order to get the full picture. The new approaches created by the leading companies in the polymer industry are remarkable and ought to be applied.

Nomenclature

A – heat transfer area, [m^2]
C_p – specific heat, [Jkg^{-1}K^{-1}]
D – diameter, [m]
D_{ci} – half coil inside diameter, [m]
D_{co} – half coil outside diameter, [m]
D_e – equivalent hydraulic diameter of heat transfer, [m]
F – fouling factor, [m^{2}kW^{-1}]
H_p – polymerization heat of reaction, [kJmol^{-1}]
h – film heat transfer coefficient, [Wm^{-2}°C^{-1}]
M – mass weight, [kg]

$\dot{m}$ – mass-flow rate, [kgs^{-1}]
N – agitation speed, [rpm]
N_{Pr} – Prandlt number (= $C_p\mu/\kappa$), [–]
N_{Re} – Reynolds number (= $D^2N\rho/\mu$), [–]
N_U – Nusselt number (= hD/κ), [–]
Q – heat transfer, [kW]
q_r – heat of reaction, [kW]
T – temperature, [°C]
t – time, [s]
U – overall heat transfer coefficient, [$Wm^{-2}°C^{-1}$]
v – velocity, [ms^{-1}]
V_v – vessel volume, [m^3]
X – thickness of the vessel wall, [m]

Greek symbols

α – cooling rate, [$°Cs^{-1}$]
Δ – difference, [–]
ζ – conversation rate of reaction, [$molm^{-3}s^{-1}$]
κ – thermal conductivity, [$Wm^{-1}°C^{-1}$]
μ – fluid viscosity, [Pa·s]
ρ – density, [kgm^{-3}]
Φ – volume flow rate, [m^3s^{-1}]

Subscripts

b – batch condition
j – jacket condition
mean – mean condition
w – wall condition

Acronyms

VCM – vinyl chloride monomer
TEMA – tubular exchanger manufacturers association

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